LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	12	15	21	rVV	405862	529955	1.62%	0.277%
2	3.146	23	27	35	rVB	233676	407485	1.25%	0.213%
3	3.493	81	86	103	rVB2	134383	351572	1.08%	0.183%
4	3.981	163	169	177	rVB3	197780	369946	1.13%	0.193%
5	4.999	337	342	350	rVB	458024	684660	2.10%	0.357%
6	5.469	415	422	433	rVB	7187361	11180023	34.24%	5.834%
7	6.205	535	547	556	rBV5	114249	461802	1.41%	0.241%
8	6.763	629	642	654	rVB2	143075	350768	1.07%	0.183%
9	7.058	684	692	704	rBV	7041334	11534838	35.32%	6.019%
10	7.187	708	714	722	rBV2	148595	464272	1.42%	0.242%
11	7.887	825	833	839	rBV	2229018	3687489	11.29%	1.924%
12	7.952	839	844	857	rVB5	227640	628387	1.92%	0.328%
13	8.246	887	894	906	rBV5	165933	471072	1.44%	0.246%
14	9.040	1022	1029	1039	rBV	4489240	7674123	23.50%	4.004%
15	10.510	1265	1279	1293	rBV	2885970	5604797	17.16%	2.925%
16	10.687	1300	1309	1316	rBV	2915396	5039890	15.43%	2.630%
17	11.263	1399	1407	1414	rBV2	269330	551091	1.69%	0.288%
18	11.393	1423	1429	1436	rBV	241774	405021	1.24%	0.211%
19	11.698	1476	1481	1494	rVB	270439	591850	1.81%	0.309%
20	13.145	1719	1727	1737	rBV	13751200	21074576	64.54%	10.997%
21	13.816	1836	1841	1847	rBV	230363	353158	1.08%	0.184%
22	14.234	1907	1912	1920	rBV2	235962	489044	1.50%	0.255%
23	14.422	1936	1944	1952	rBV	1023484	1712395	5.24%	0.894%
24	14.516	1953	1960	1966	rBV	4580148	7049842	21.59%	3.679%
25	16.004	2207	2213	2221	rBV	10774479	15534500	47.57%	8.106%
26	16.857	2354	2358	2366	rVB2	651280	961987	2.95%	0.502%
27	17.016	2381	2385	2394	rBV5	408696	817044	2.50%	0.426%
28	17.263	2422	2427	2437	rVB	5107229	7905528	24.21%	4.125%
29	17.533	2470	2473	2476	rBV2	274603	348586	1.07%	0.182%
30	18.163	2576	2580	2586	rBV	2002698	2803715	8.59%	1.463%
31	18.857	2696	2698	2702	rBV2	603026	692596	2.12%	0.361%
32	19.398	2786	2790	2798	rBV	1640063	2399056	7.35%	1.252%
33	19.822	2857	2862	2868	rVB	19259623	23835296	72.99%	12.438%
34	21.351	3117	3122	3130	rVB	4923355	7214507	22.09%	3.765%
35	21.486	3139	3145	3160	rBV	19037105	32654940	100.00%	17.040%
36	21.904	3210	3216	3223	rVB	5156053	9006943	27.58%	4.700%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.774	3531	3534	3542	rVB2	3254303	5795352	17.75%	3.024%

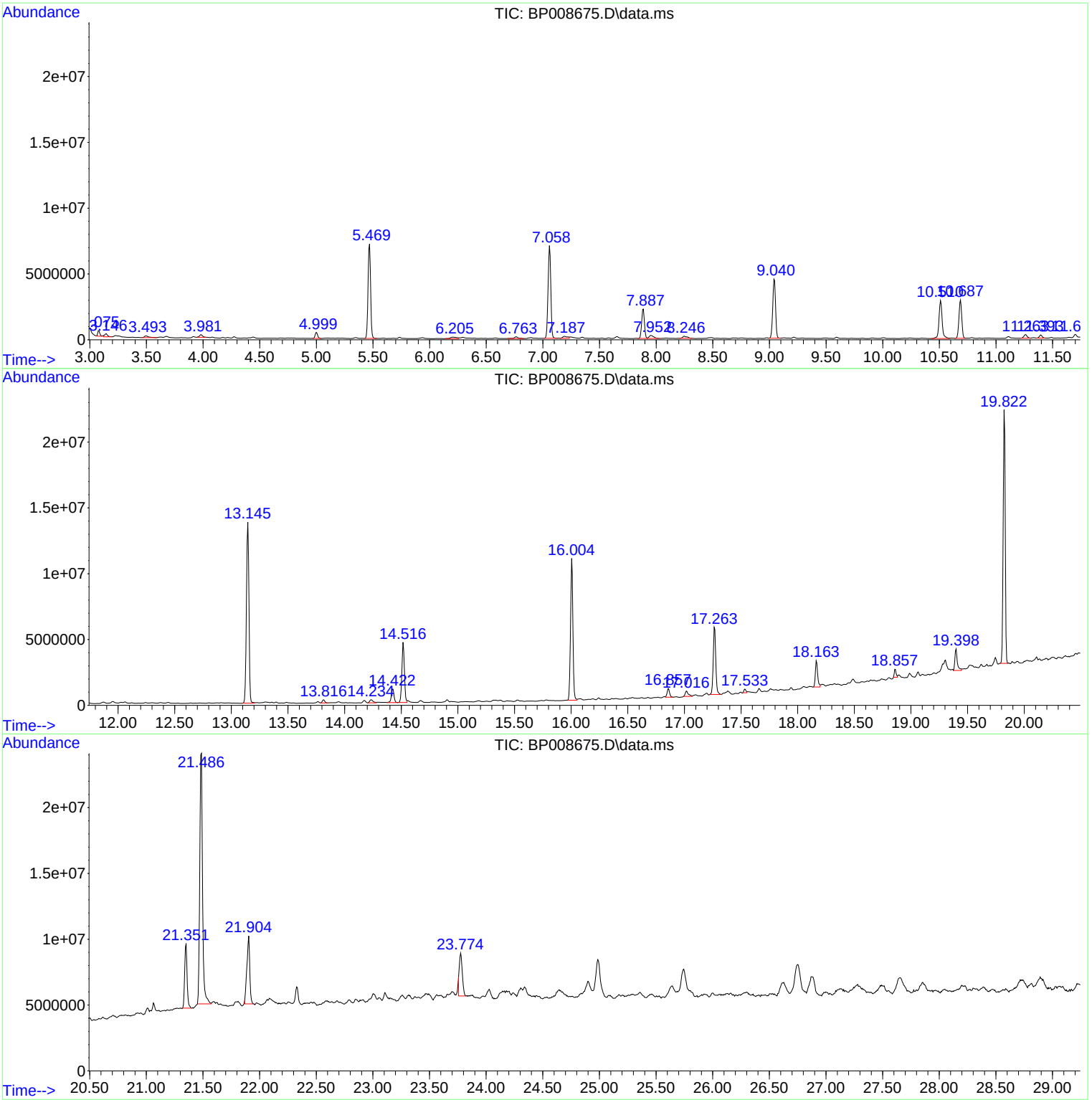
Sum of corrected areas: 191638106

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

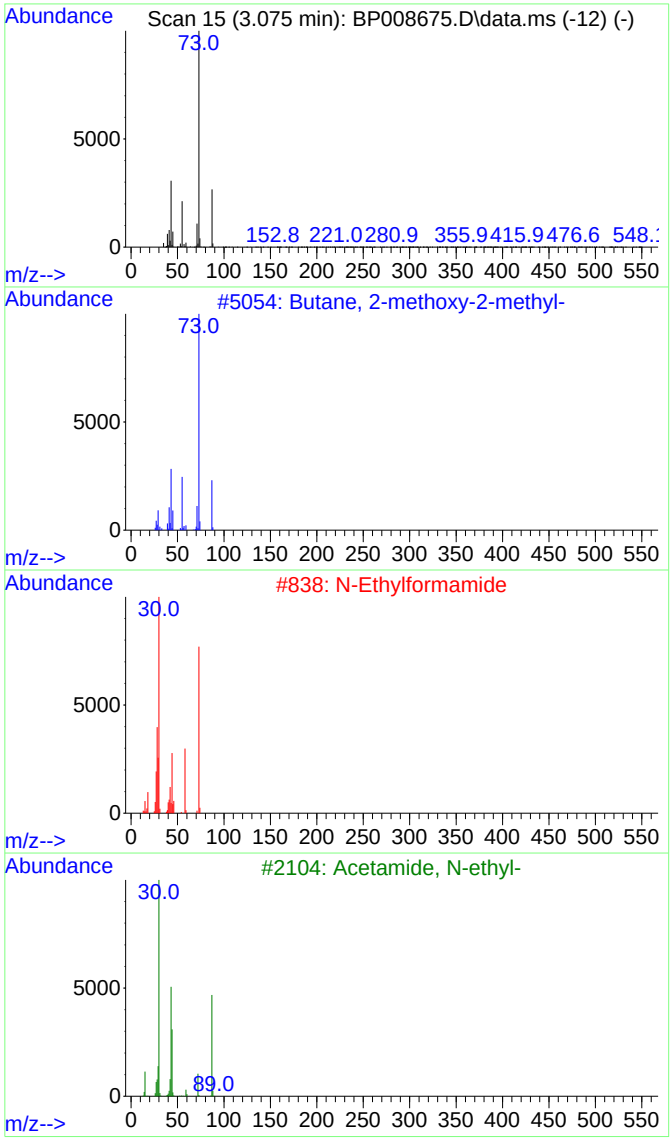
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

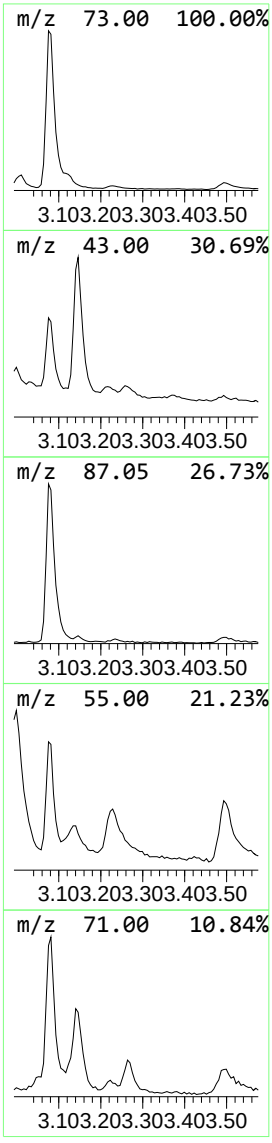
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	2.87 ng	529955	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

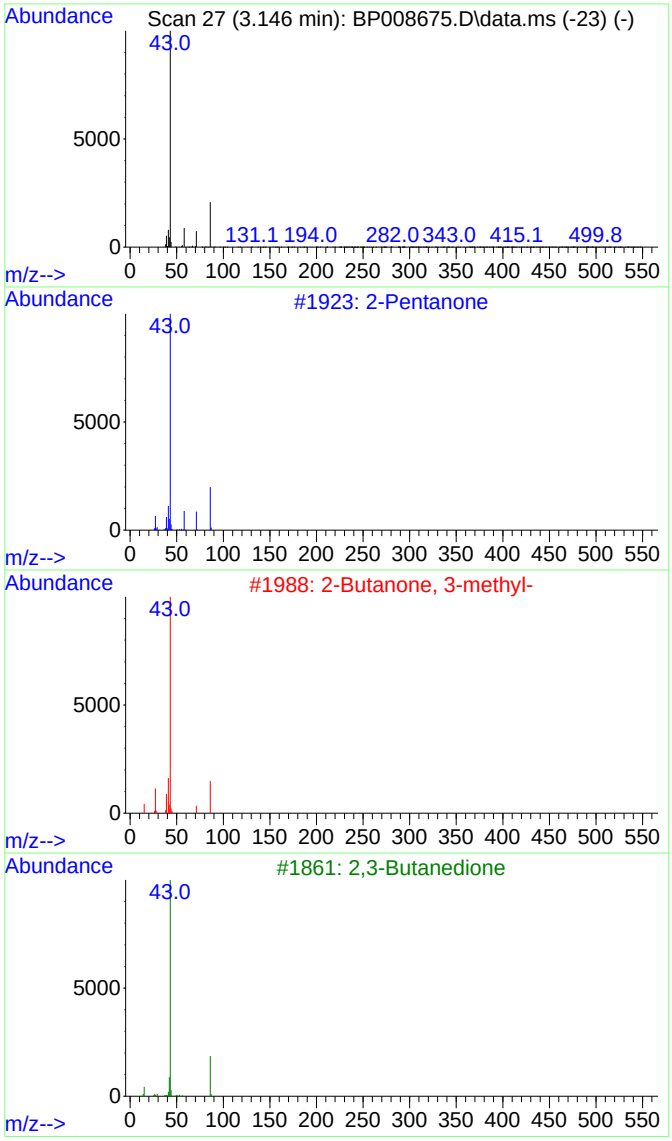
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

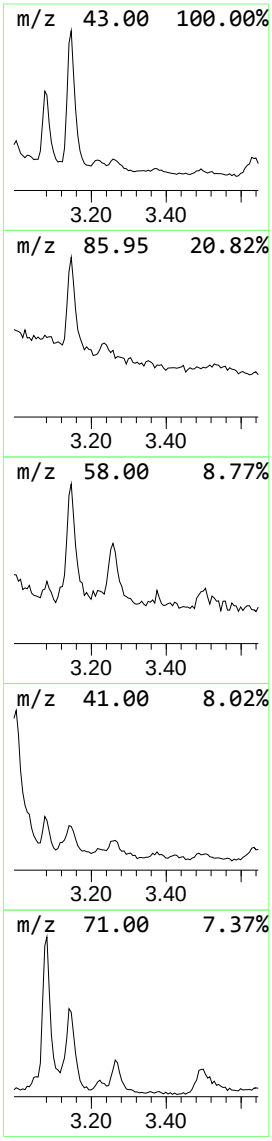
****

Peak Number 2 2-Pentanone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.146	2.21 ng	407485	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	72
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	2,3-Butanedione	86	C4H6O2	000431-03-8	9
4	Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	5
5	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

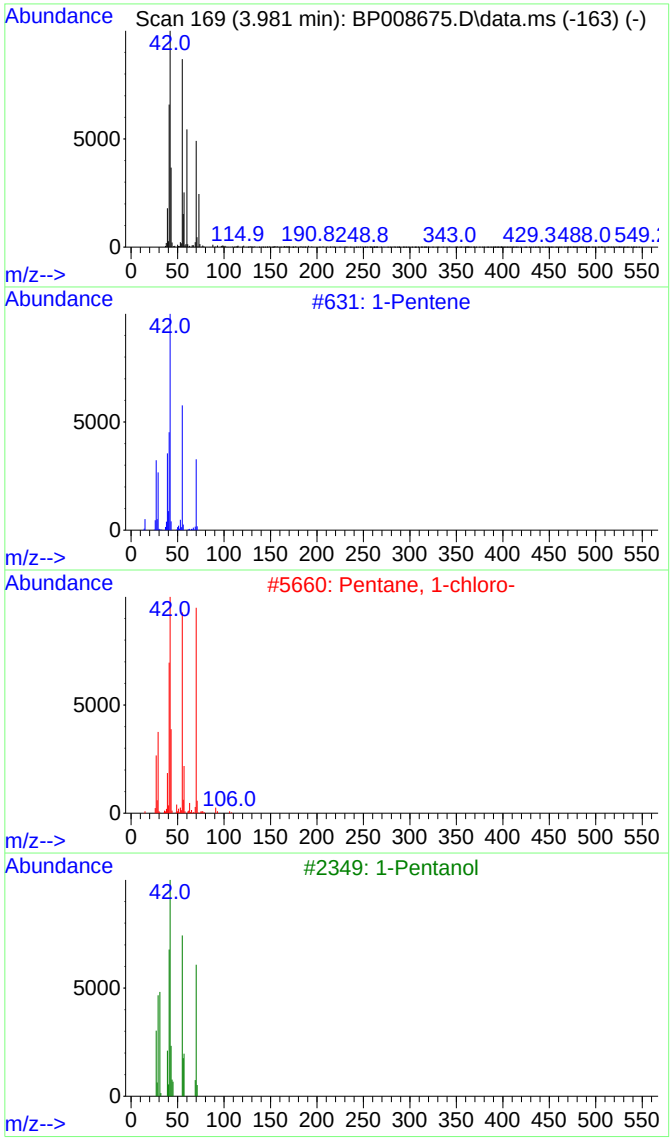
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

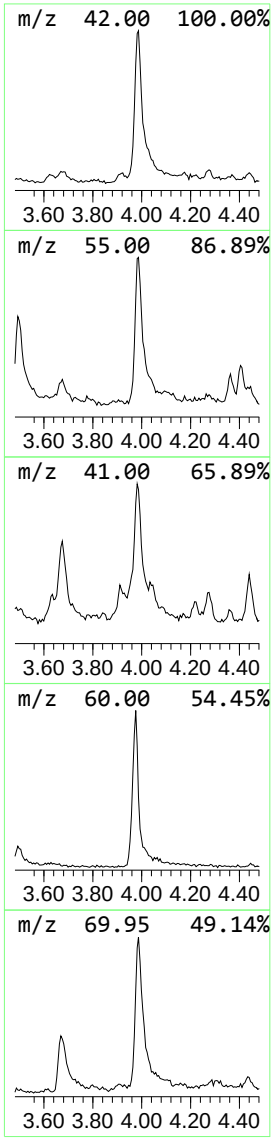
****

Peak Number 3 1-Pentene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	2.01 ng	369946	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	50
2	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	50
3	1-Pentanol	88	C5H12O	000071-41-0	50
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	47
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

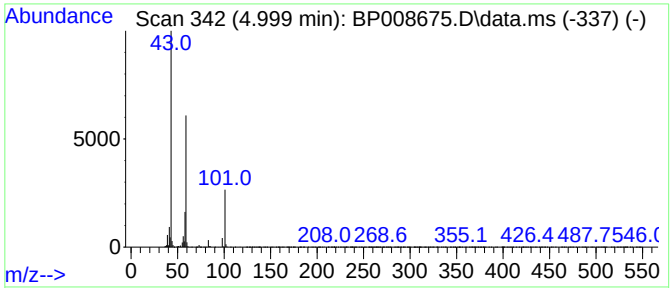
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

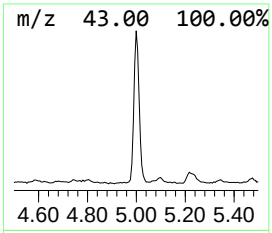
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

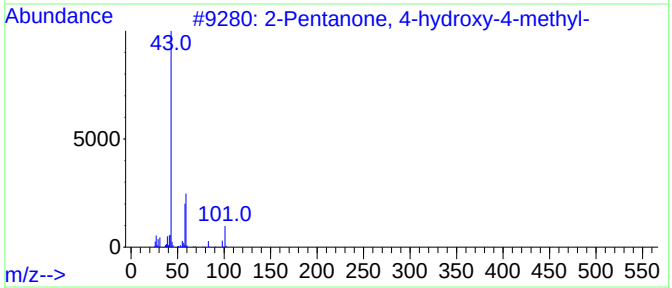
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

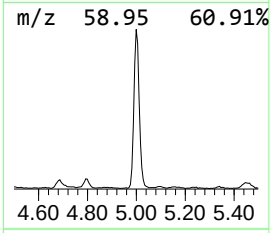
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	3.71 ng	684660	1,4-Dichlorobenzene-d4	7.887

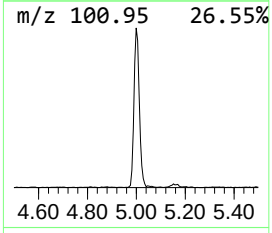
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	1,2-Butanediol	90	C4H10O2	000584-03-2	17

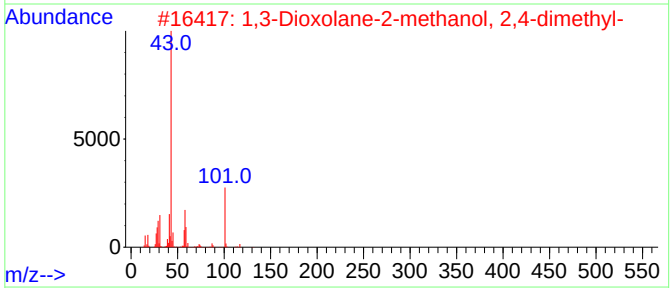


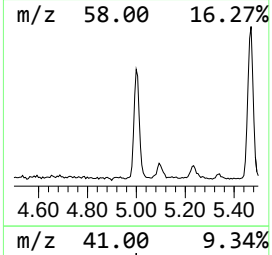


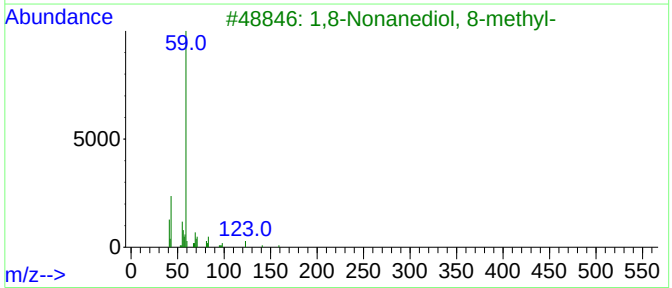


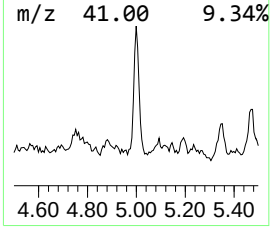












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

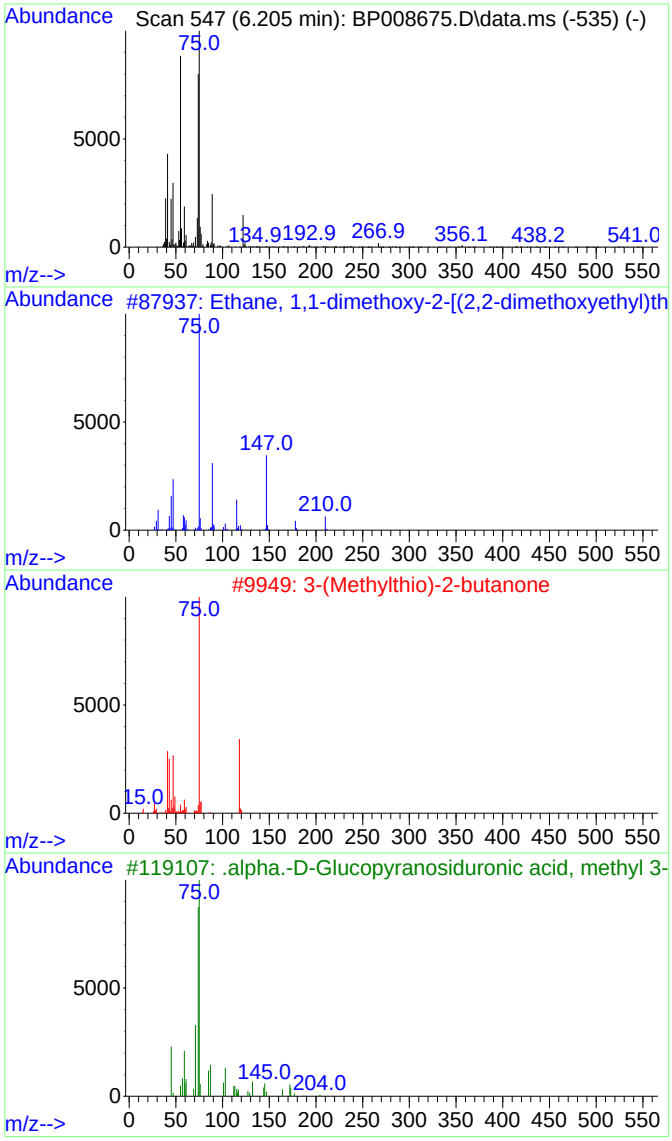
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

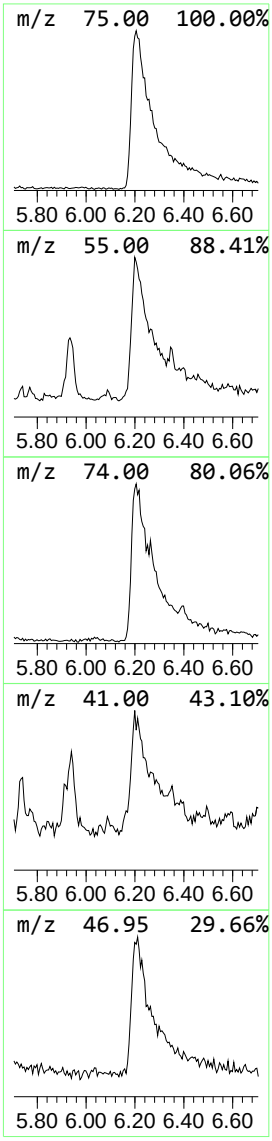
****

Peak Number 5 unknown6.205 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.205	2.50 ng	461802	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-dimethoxy-2-[(2,2-di...	210	C8H18O4S	078102-16-6	38
2	3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	35
3	.alpha.-D-Glucopyranosiduronic a...	236	C9H16O7	031506-19-1	32
4	Ethane, 1,1'-oxybis[2,2-dimethoxy-	194	C8H18O5	078082-46-9	32
5	Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

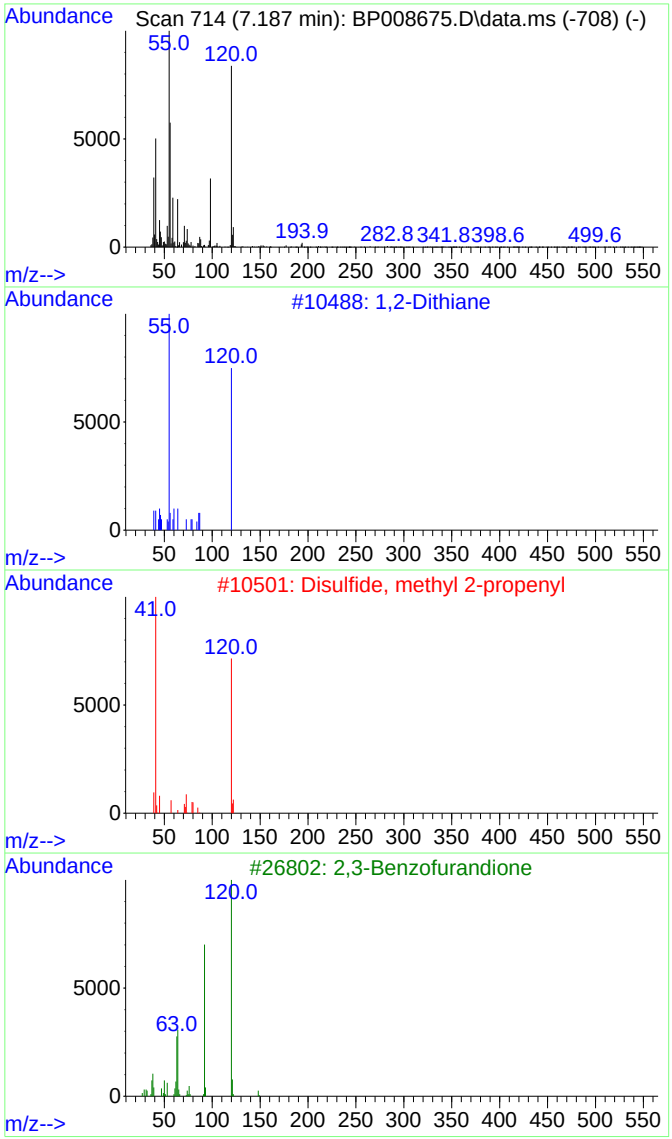
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

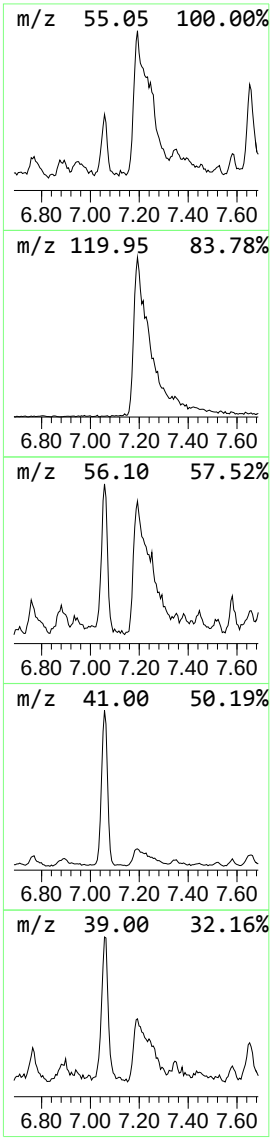
****

Peak Number 6 unknown7.187 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.187	2.52 ng	464272	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dithiane	120	C4H8S2	000505-20-4	37
2	Disulfide, methyl 2-propenyl	120	C4H8S2	002179-58-0	27
3	2,3-Benzofurandione	148	C8H4O3	004732-72-3	17
4	Benzoic acid, 4-amino-, 2,2,6,6-...	290	C16H22N2O3	1000261-13-4	16
5	Silanol, trimethyl-, nitrate	135	C3H9NO3Si	018026-82-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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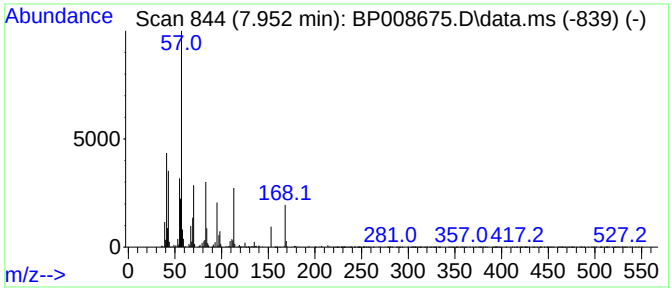
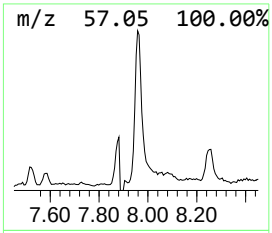
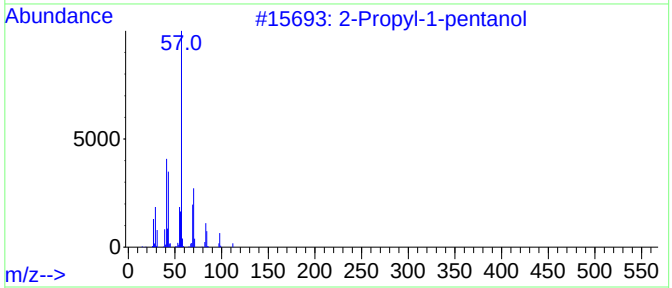
Peak Number 7 unknown7.952 Concentration Rank 8

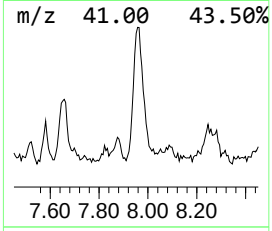
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.952	3.41 ng	628387	1,4-Dichlorobenzene-d4	7.887

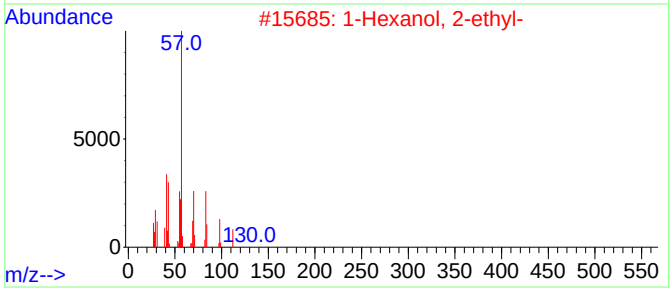
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	35
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	32
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	22
5	2,2-Dimethylhex-4-enylamine	127	C8H17N	133885-74-2	16

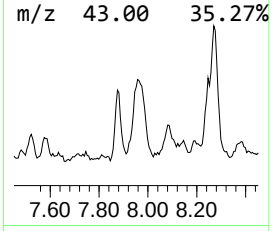


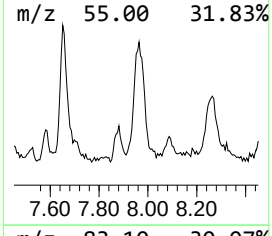


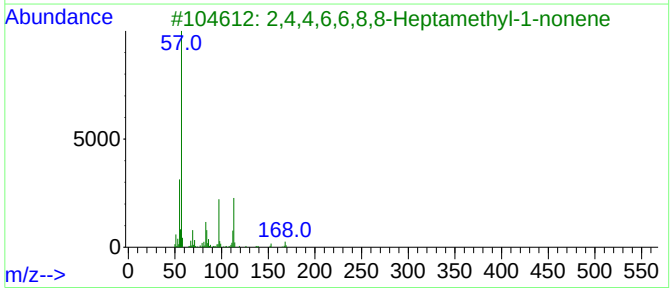


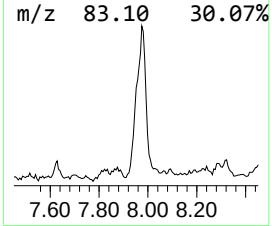












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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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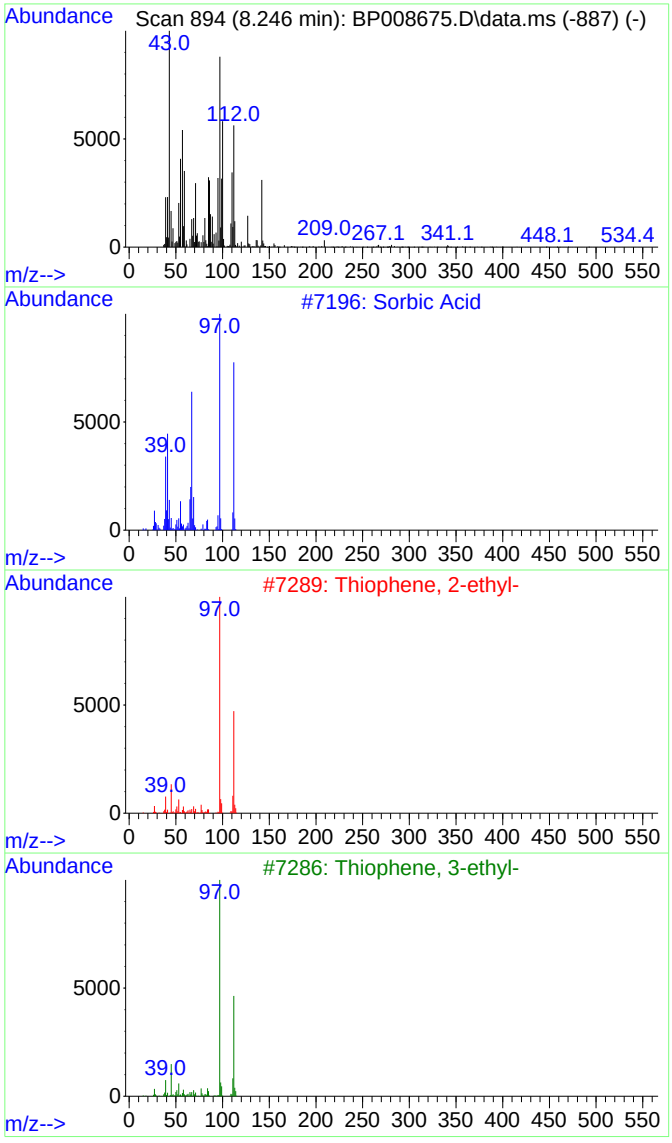
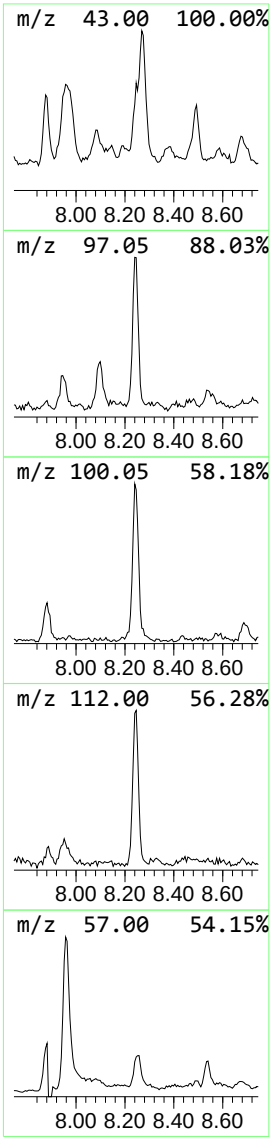
Peak Number 8 unknown8.246 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.246	2.55 ng	471072	1,4-Dichlorobenzene-d4	7.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sorbic Acid	112	C6H8O2	000110-44-1	30
2	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	27
3	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	27
4	3-Hexene-2,5-dione	112	C6H8O2	004436-75-3	27
5	3-Thiopheneacetic acid	142	C6H6O2S	006964-21-2	25





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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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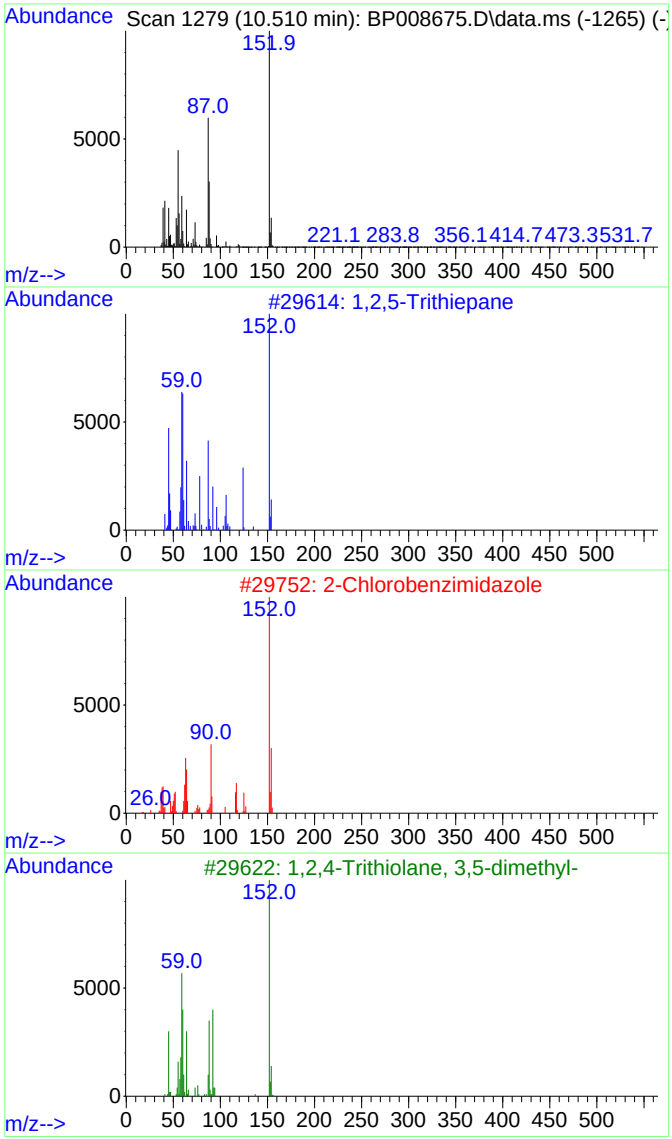
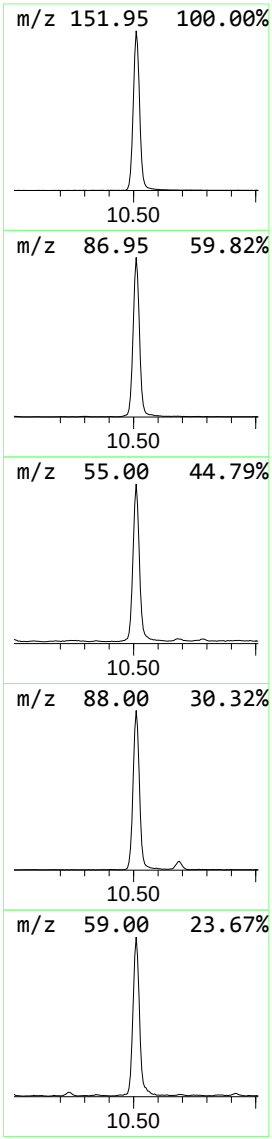
Peak Number 9 unknown10.510 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.510	22.24 ng	5604800	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	40
2	2-Chlorobenzimidazole	152	C7H5ClN2	004857-06-1	35
3	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	33
4	Thiophene, 2,3-dichloro-	152	C4H2Cl2S	017249-79-5	25
5	2-Heptenoic acid, methyl ester	142	C8H14O2	022104-69-4	18





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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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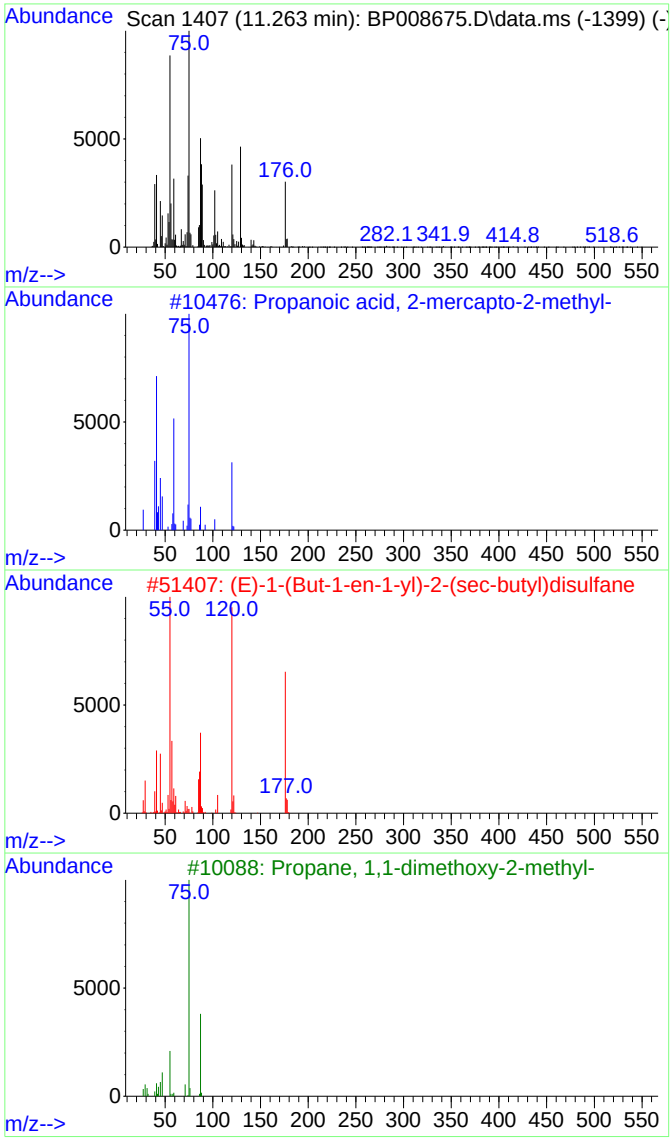
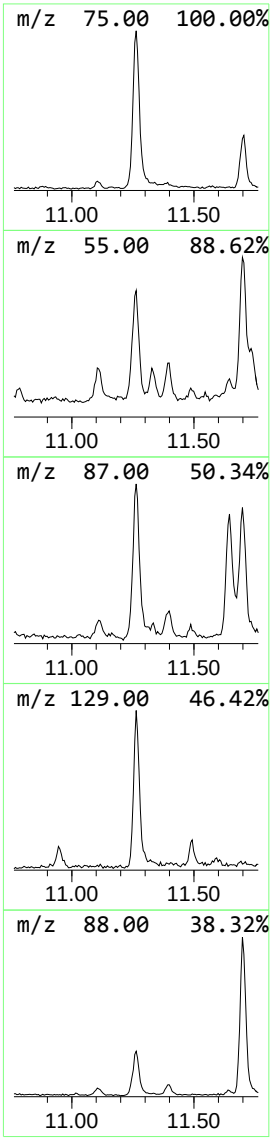
Peak Number 10 unknown11.263 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	2.19 ng	551091	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-mercapto-2-met...	120	C4H8O2S	004695-31-2	35
2	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	25
3	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	22
4	Glucopyranoside, methyl 4-deoxy-...	266	C11H19FO6	030694-48-5	22
5	Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	18





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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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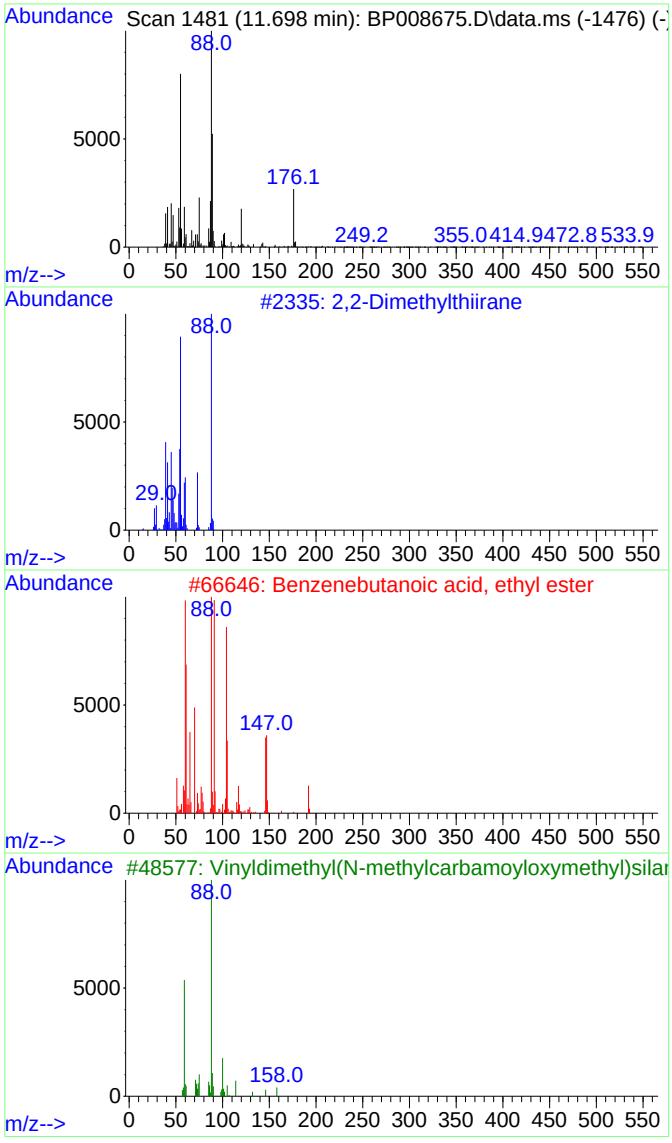
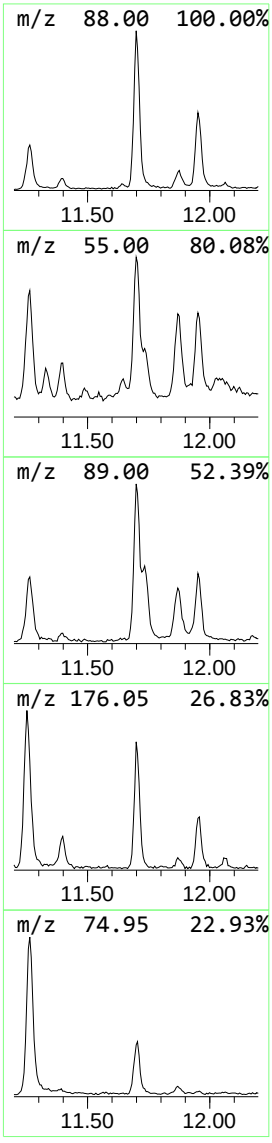
Peak Number 11 unknown11.698 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	2.35 ng	591850	Naphthalene-d8	10.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	38
2	Benzenebutanoic acid, ethyl ester	192	C12H16O2	010031-93-3	35
3	Vinyldimethyl(N-methylcarbamoylo...	173	C7H15NO2Si	120491-43-2	32
4	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	30
5	Undecanoic acid, 2-methyl-, meth...	214	C13H26O2	055955-69-6	27





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Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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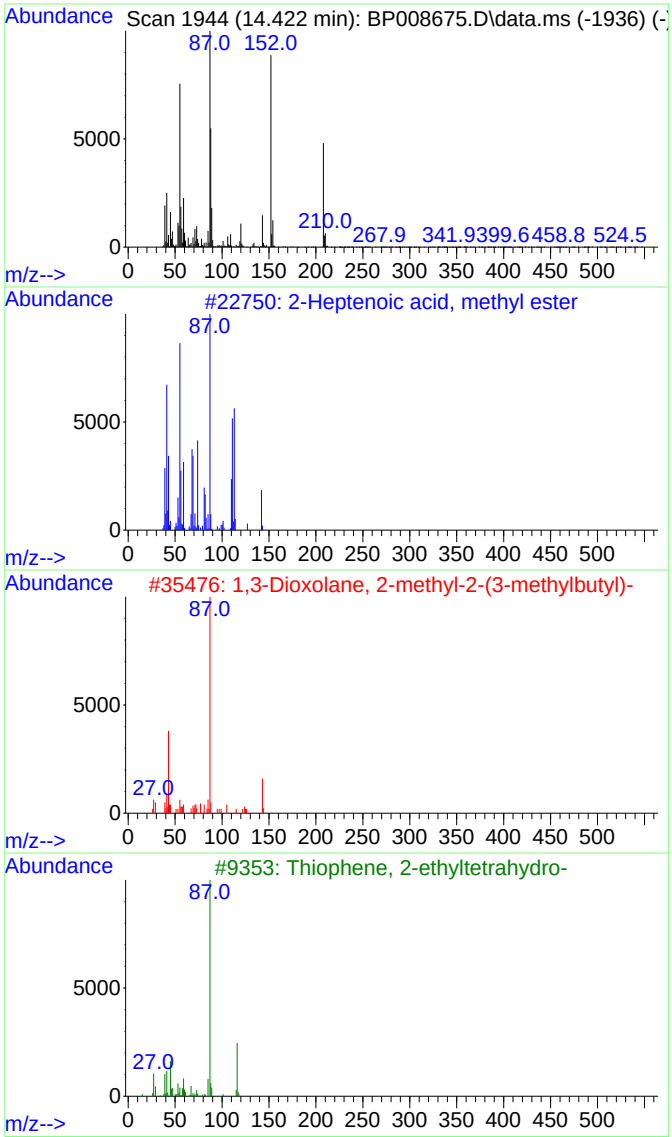
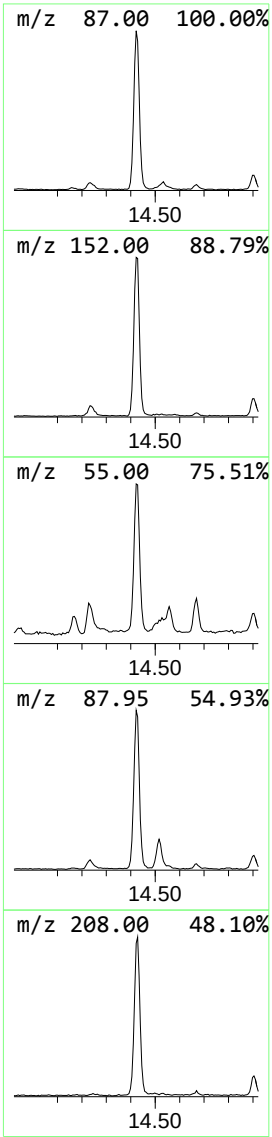
Peak Number 12 unknown14.422 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	4.86 ng	1712400	Acenaphthene-d10	14.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptenoic acid, methyl ester	142	C8H14O2	022104-69-4	22
2	1,3-Dioxolane, 2-methyl-2-(3-met...	158	C9H18O2	014447-30-4	22
3	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	14
4	2-[2-[2-[2-[2-[2-[2-(2-Acetyl...	498	C22H42O12	1010351-90-5	14
5	2-O-Methyl-d-xylose	164	C6H12O5	1000130-01-3	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
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Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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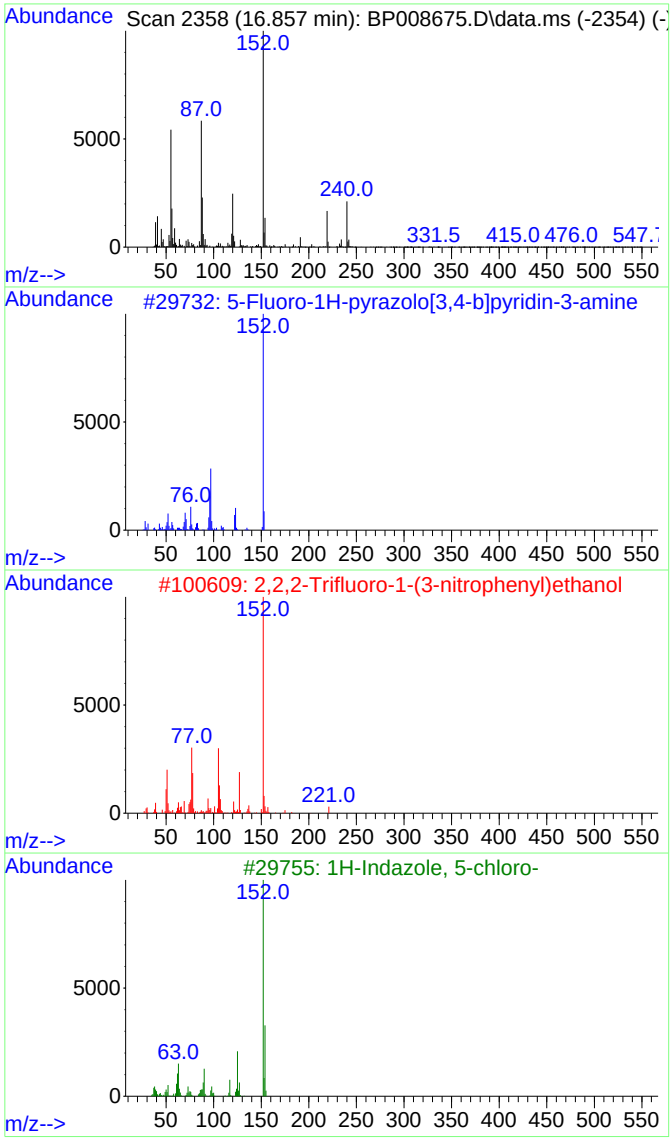
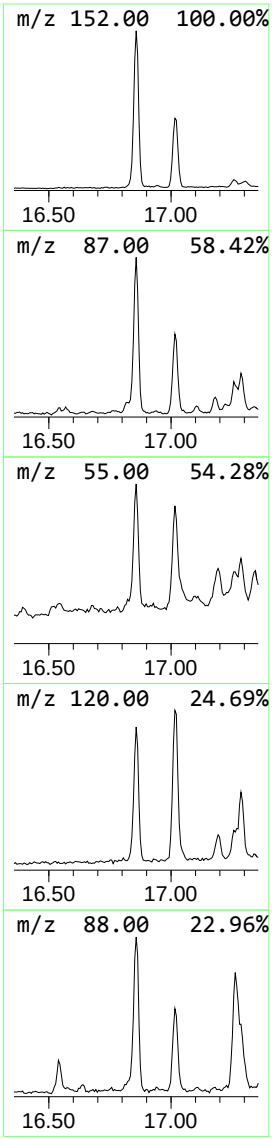
Peak Number 13 unknown16.857 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.857	2.43 ng	961987	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-1H-pyrazolo[3,4-b]pyrid...	152	C6H5FN4	1034667-22-5	12
2	2,2,2-Trifluoro-1-(3-nitrophenyl...	221	C8H6F3NO3	000453-77-0	10
3	1H-Indazole, 5-chloro-	152	C7H5ClN2	000698-26-0	10
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	10
5	1,3-Dioxolane, 4-methyl-2-pentad...	298	C19H38O2	054950-56-0	9





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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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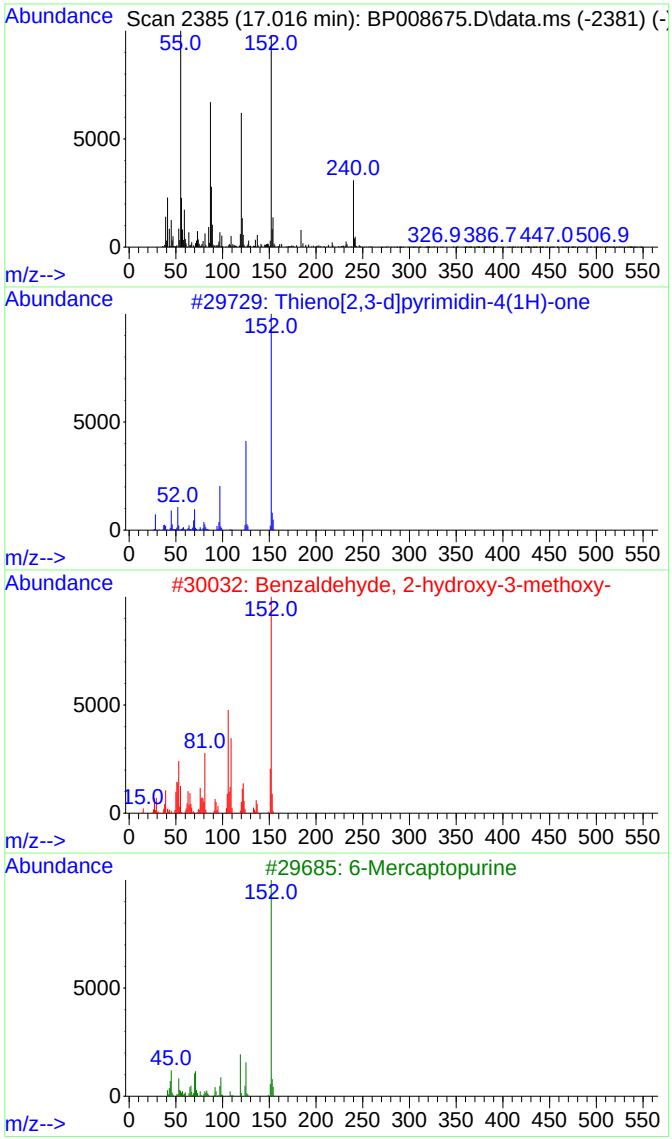
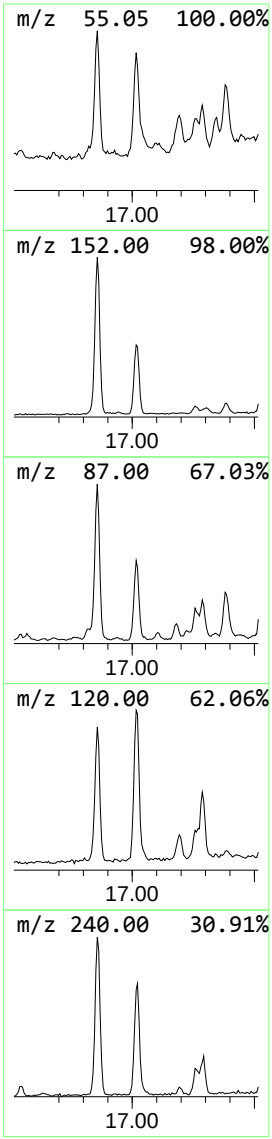
Peak Number 14 unknown17.016 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.016	2.07 ng	817044	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thieno[2,3-d]pyrimidin-4(1H)-one	152	C6H4N2OS	014080-50-3	25
2	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	22
3	6-Mercaptopurine	152	C5H4N4S	000050-44-2	22
4	3,4-Diaminobenzoic acid	152	C7H8N2O2	000619-05-6	14
5	l-Allylglycine, N-propargyloxyca...	235	C12H13NO4	1000325-13-1	14





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Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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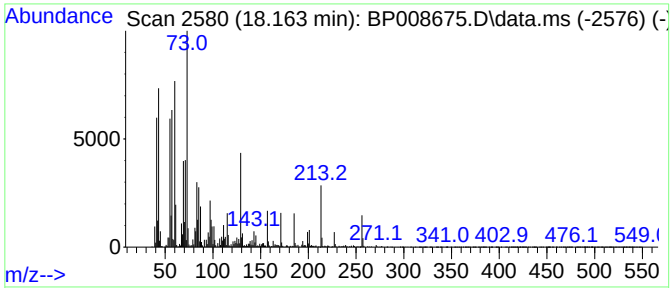
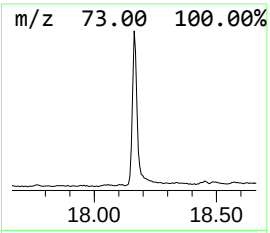
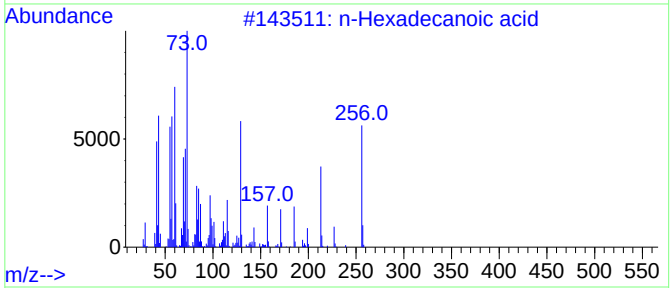
Peak Number 15 n-Hexadecanoic acid Concentration Rank 4

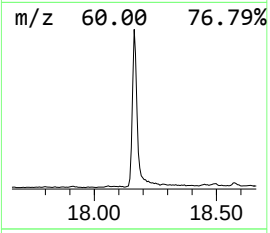
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	7.09 ng	2803720	Phenanthrene-d10	17.263

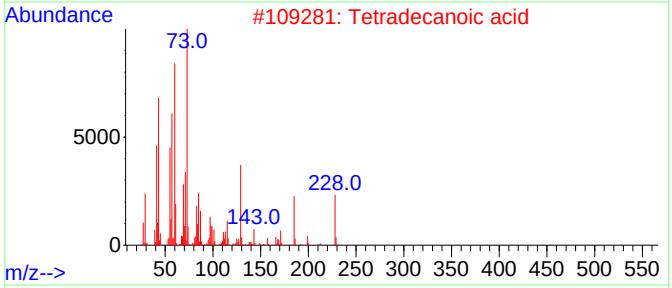
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76

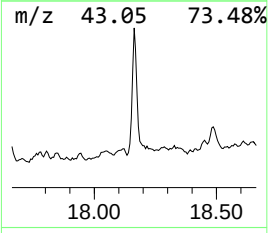


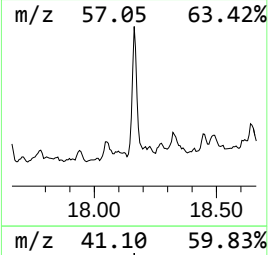


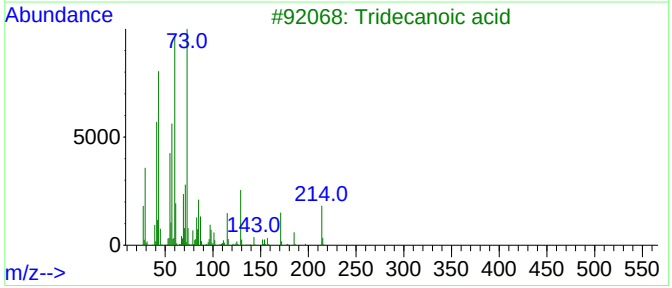


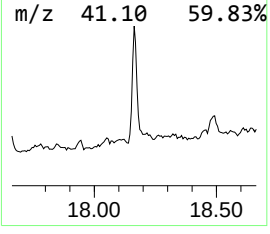












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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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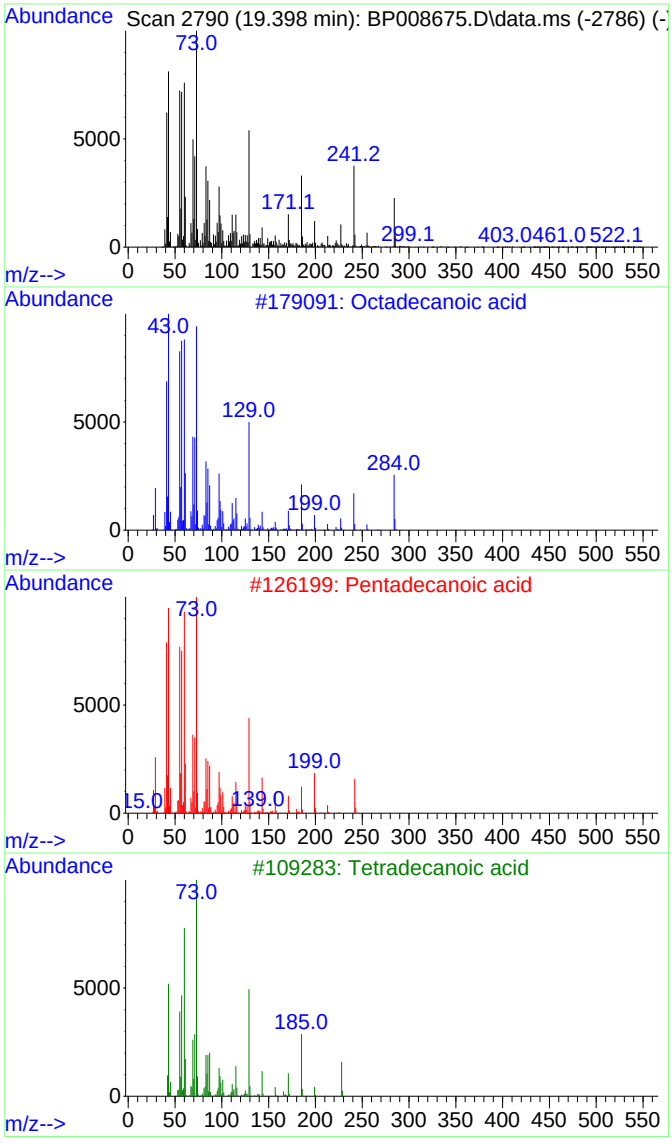
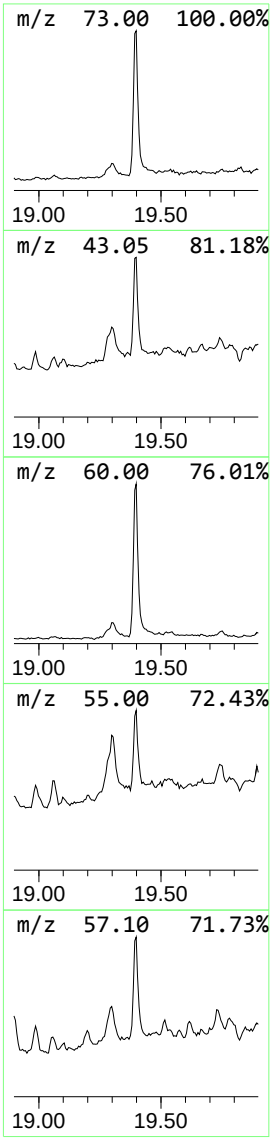
Peak Number 16 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	6.65 ng	2399060	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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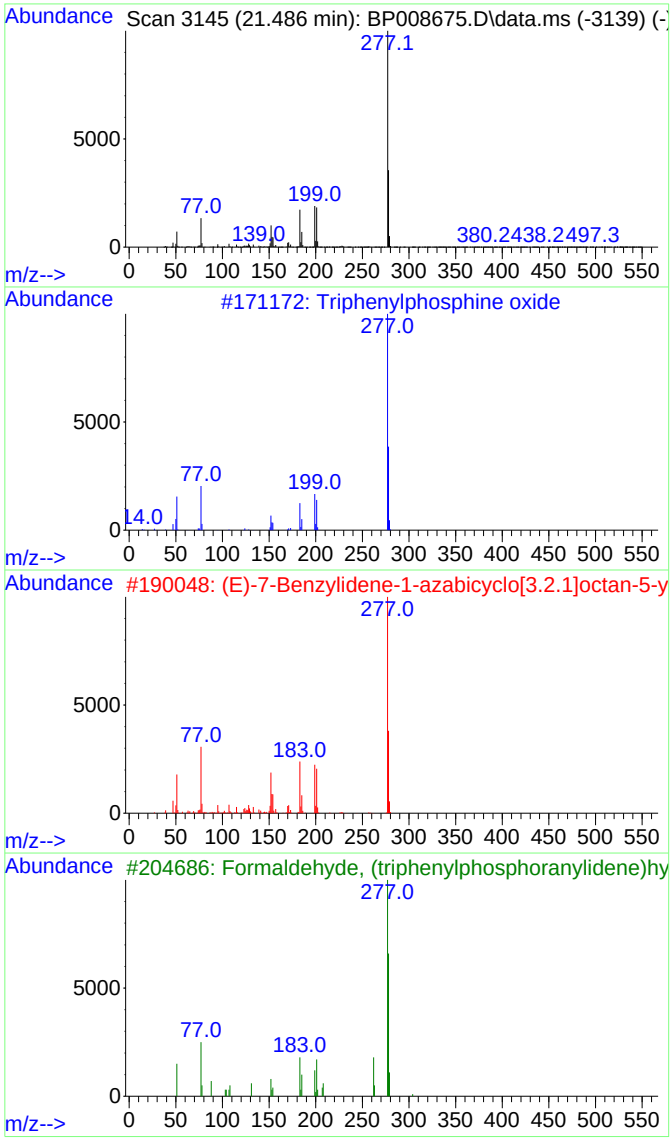
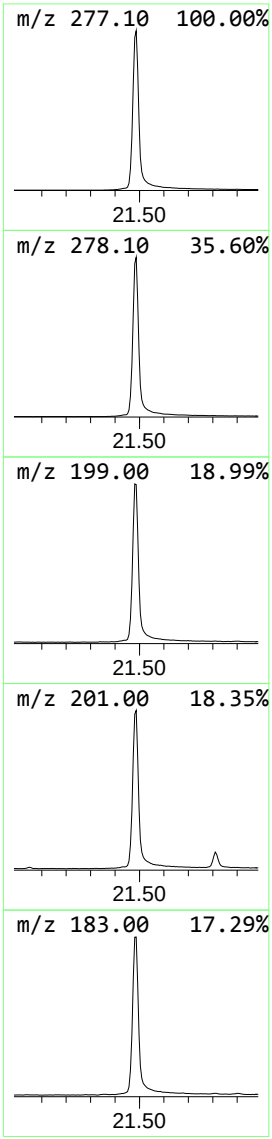
Peak Number 17 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.486	90.53 ng	32654900	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5	Oxoprophines	277	C17H11NO3	1000128-51-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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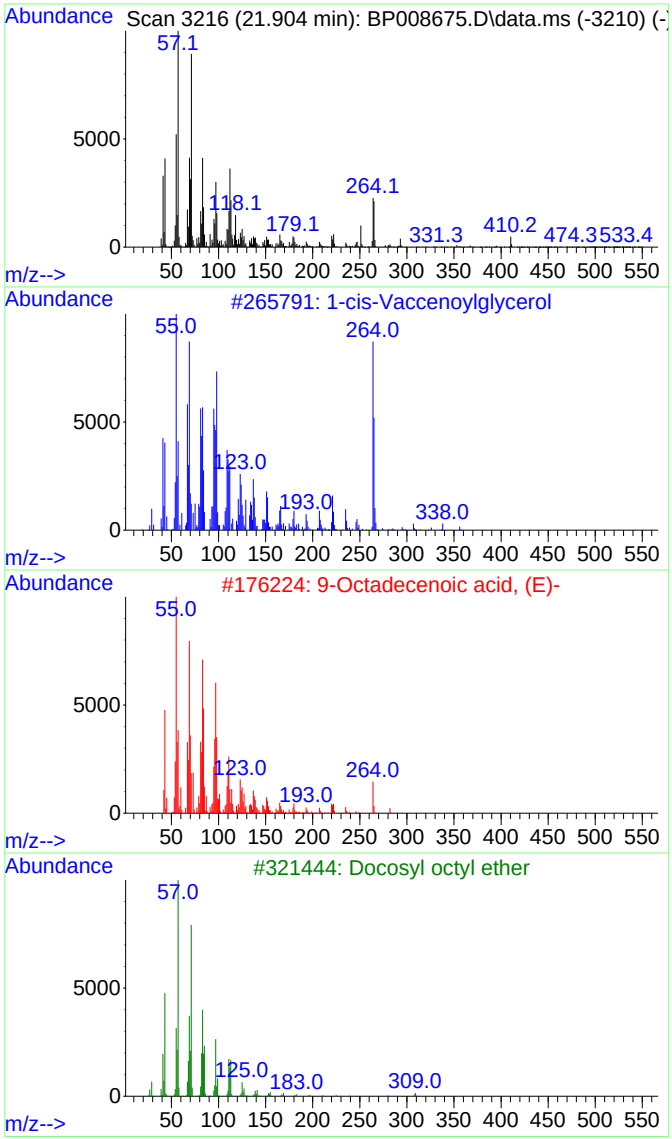
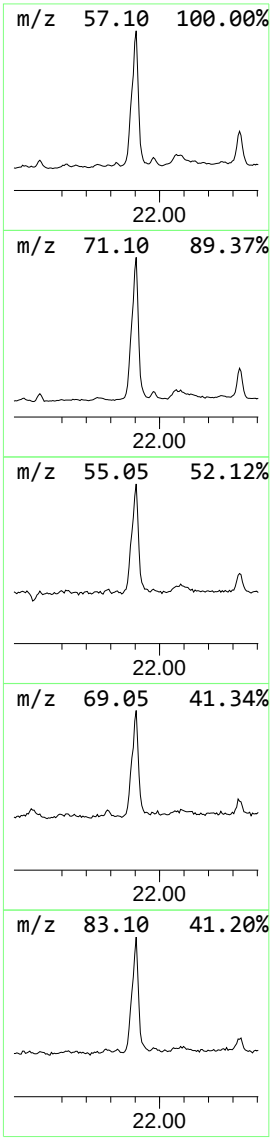
Peak Number 18 1-cis-Vaccenoylglycerol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.904	24.97 ng	9006940	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-cis-Vaccenoylglycerol	356	C21H40O4	020379-67-3	59
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	53
3	Docosyl octyl ether	438	C30H62O	1000406-38-9	53
4	Eicosyl octyl ether	410	C28H58O	1000406-38-8	50
5	9-Octadecenoic acid (Z)-, pentyl...	352	C23H44O2	000142-57-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010422\
Data File : BP008675.D
Acq On : 04 Jan 2022 22:40
Operator : CG/JU
Sample : M5338-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-7-(4.5-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.075	2.9	ng	529955	1	7.887	3687490	20.0
2-Pentanone	3.146	2.2	ng	407485	1	7.887	3687490	20.0
1-Pentene	3.981	2.0	ng	369946	1	7.887	3687490	20.0
2-Pentanone, 4-...	4.999	3.7	ng	684660	1	7.887	3687490	20.0
unknown6.205	6.205	2.5	ng	461802	1	7.887	3687490	20.0
unknown7.187	7.187	2.5	ng	464272	1	7.887	3687490	20.0
unknown7.952	7.952	3.4	ng	628387	1	7.887	3687490	20.0
unknown8.246	8.246	2.5	ng	471072	1	7.887	3687490	20.0
unknown10.510	10.510	22.2	ng	5604800	2	10.687	5039890	20.0
unknown11.263	11.263	2.2	ng	551091	2	10.687	5039890	20.0
unknown11.698	11.698	2.4	ng	591850	2	10.687	5039890	20.0
unknown14.422	14.422	4.9	ng	1712400	3	14.516	7049840	20.0
unknown16.857	16.857	2.4	ng	961987	4	17.263	7905530	20.0
unknown17.016	17.016	2.1	ng	817044	4	17.263	7905530	20.0
n-Hexadecanoic ...	18.163	7.1	ng	2803720	4	17.263	7905530	20.0
Octadecanoic acid	19.398	6.7	ng	2399060	5	21.351	7214510	20.0
Triphenylphosph...	21.486	90.5	ng	32654900	5	21.351	7214510	20.0
1-cis-Vaccenoyl...	21.904	25.0	ng	9006940	5	21.351	7214510	20.0