LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

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-BP011422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	7	11	32	rVB	689150	1171444	10.27%	1.167%
2	5.434	410	416	431	rBV	1627711	2751213	24.13%	2.740%
3	7.028	680	687	702	rBV	1737465	3048881	26.74%	3.037%
4	7.852	818	827	837	rBV	1375233	2257628	19.80%	2.249%
5	9.010	1017	1024	1036	rBV	1099620	1921941	16.85%	1.914%
6	10.652	1293	1303	1320	rBV	1797374	3317243	29.09%	3.304%
7	13.116	1715	1722	1733	rBV	3533846	5253979	46.07%	5.233%
8	13.328	1753	1758	1764	rVB	95951	135663	1.19%	0.135%
9	14.398	1936	1940	1945	rVB	154761	206378	1.81%	0.206%
10	14.493	1949	1956	1963	rBV	3002945	4615167	40.47%	4.597%
11	15.351	2098	2102	2108	rVB	219609	290470	2.55%	0.289%
12	15.763	2166	2172	2177	rBV	79788	129333	1.13%	0.129%
13	15.987	2204	2210	2218	rBV	2650065	3973771	34.85%	3.958%
14	16.222	2245	2250	2253	rBV	279646	434785	3.81%	0.433%
15	16.404	2278	2281	2288	rVB	105008	135384	1.19%	0.135%
16	17.016	2381	2385	2390	rBV	265146	332727	2.92%	0.331%
17	17.069	2390	2394	2404	rVB	128330	236218	2.07%	0.235%
18	17.251	2418	2425	2429	rBV	3739861	5556192	48.72%	5.534%
19	17.292	2429	2432	2436	rVB	274670	360548	3.16%	0.359%
20	17.381	2444	2447	2453	rVB	96732	151456	1.33%	0.151%
21	17.757	2507	2511	2515	rBV	270759	362488	3.18%	0.361%
22	17.798	2515	2518	2526	rVB2	550273	700880	6.15%	0.698%
23	17.928	2535	2540	2546	rBV	6273713	7537894	66.10%	7.508%
24	18.145	2574	2577	2584	rBV2	280735	456197	4.00%	0.454%
25	18.428	2622	2625	2629	rBV	211969	249515	2.19%	0.249%
26	18.586	2649	2652	2657	rBV4	96318	172004	1.51%	0.171%
27	19.028	2722	2727	2730	rBV	8772839	11403502	100.00%	11.359%
28	19.063	2730	2733	2737	rVB2	8847510	10218347	89.61%	10.178%
29	19.186	2750	2754	2760	rVB	2920319	3305318	28.99%	3.292%
30	19.263	2760	2767	2776	rBV	1311011	2612950	22.91%	2.603%
31	19.610	2822	2826	2835	rVB	771149	1317221	11.55%	1.312%
32	19.810	2855	2860	2865	rBV	5978408	7685054	67.39%	7.655%
33	20.151	2915	2918	2923	rVB3	405563	530399	4.65%	0.528%
34	20.416	2960	2963	2969	rBV2	421050	530809	4.65%	0.529%
35	21.057	3069	3072	3078	rVB3	472952	600587	5.27%	0.598%
36	21.345	3116	3121	3125	rBV	3904965	5085242	44.59%	5.065%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

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-BP011422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.463	3136	3141	3146	rBV	4684673	6591098	57.80%	6.565%
38	23.768	3528	3533	3542	rVB2	2288394	4753124	41.68%	4.735%

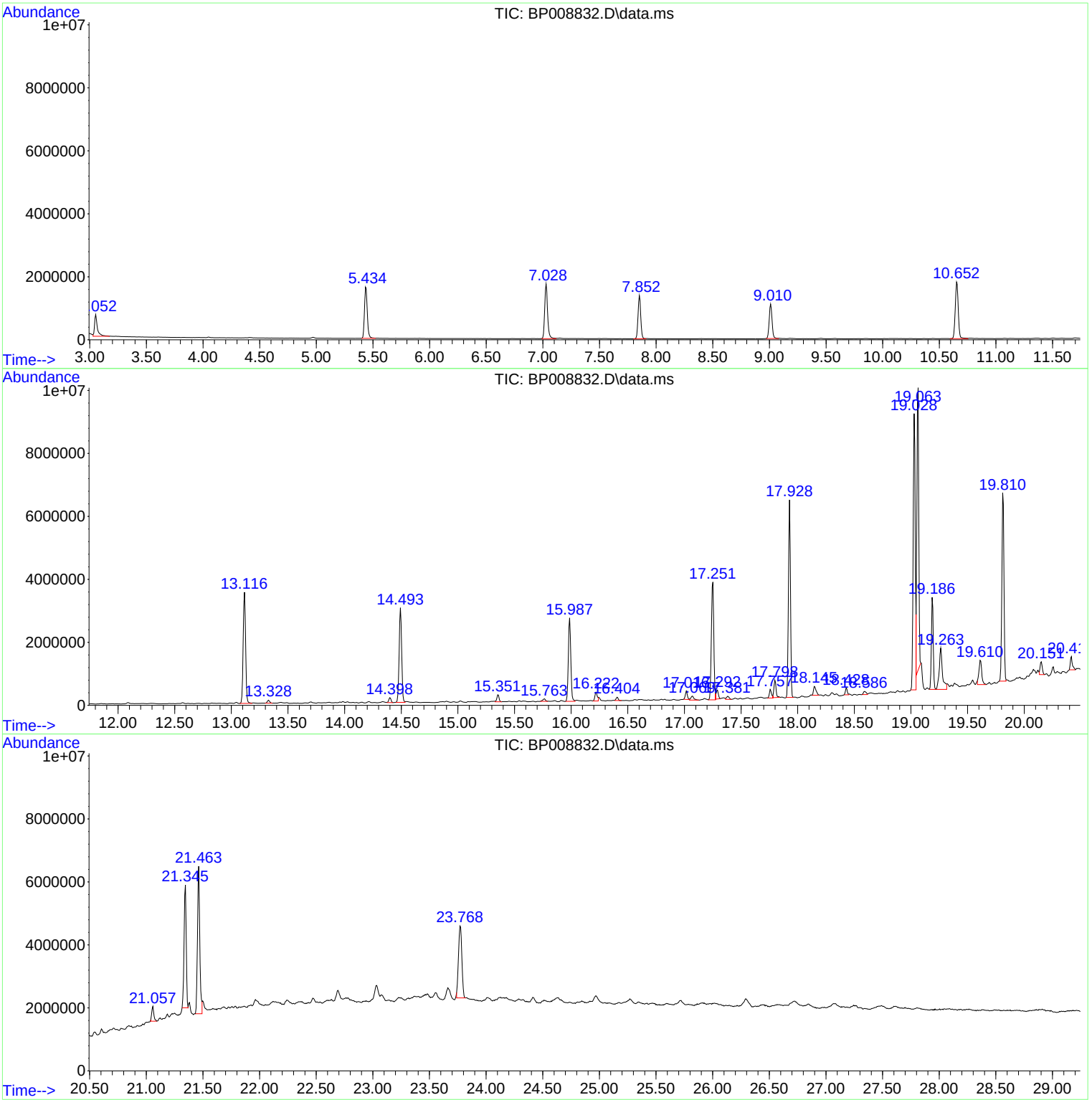
Sum of corrected areas: 100393050

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

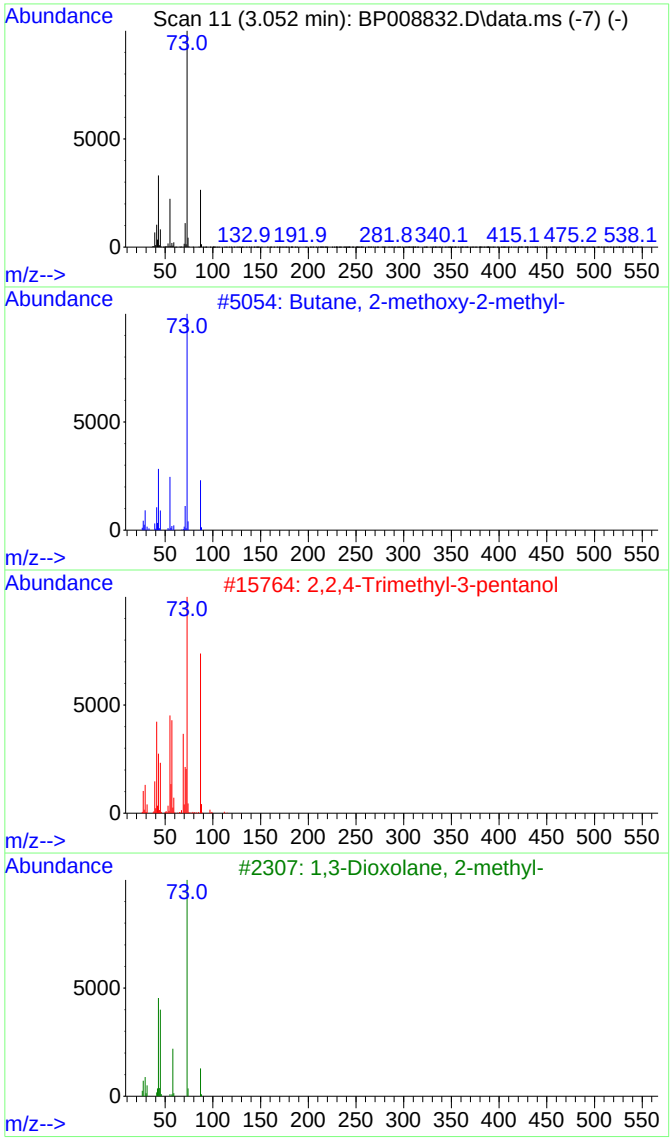
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

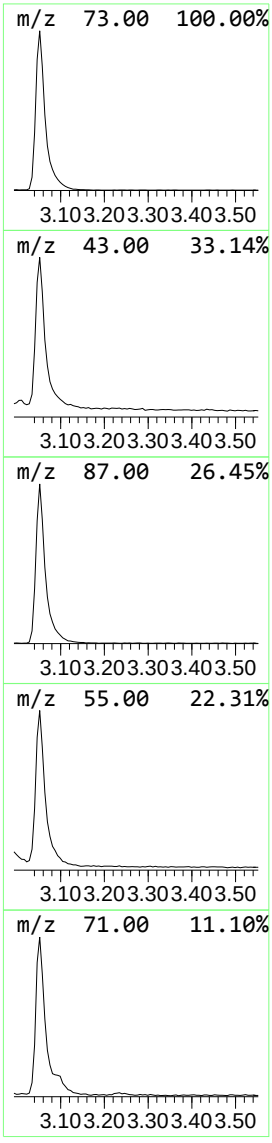
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	10.38 ng	1171440	1,4-Dichlorobenzene-d4	7.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

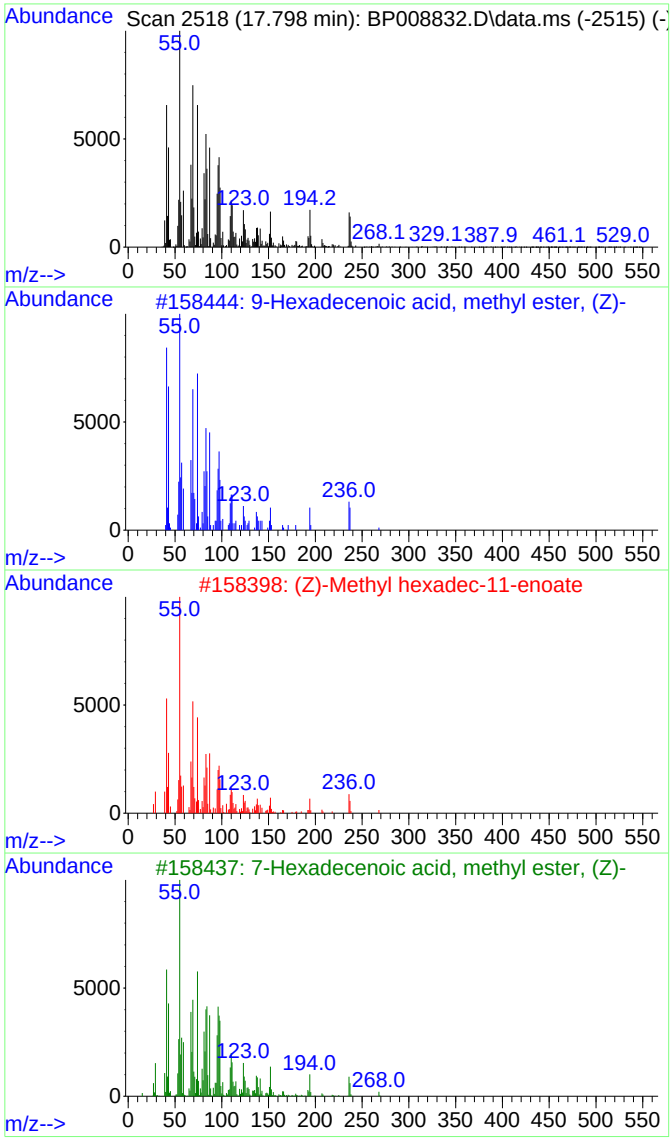
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

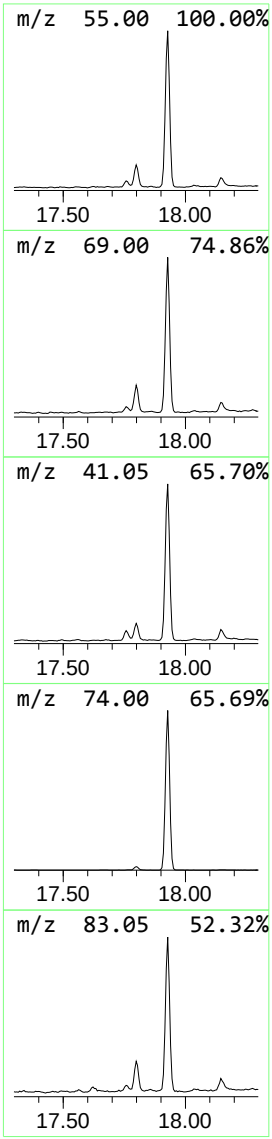
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9-Hexadecenoic acid, methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.798	2.52 ng	700880	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2	(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	96
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	95
4	6-Pentadecenoic acid, 13-methyl-...	268	C17H32O2	1000505-96-4	94
5	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

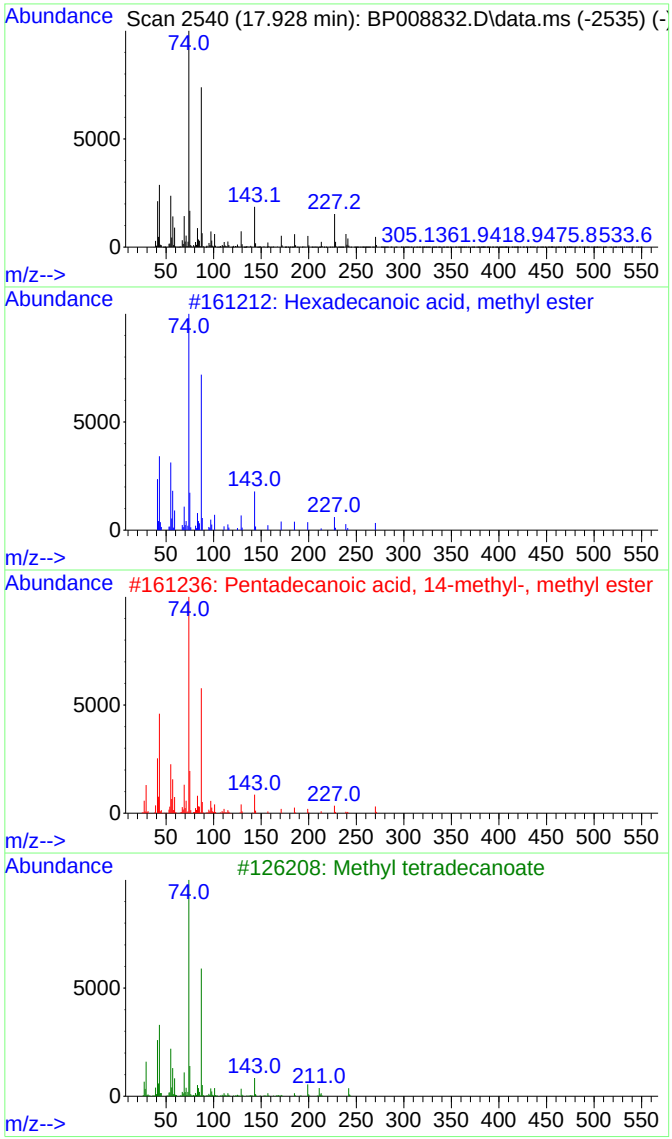
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

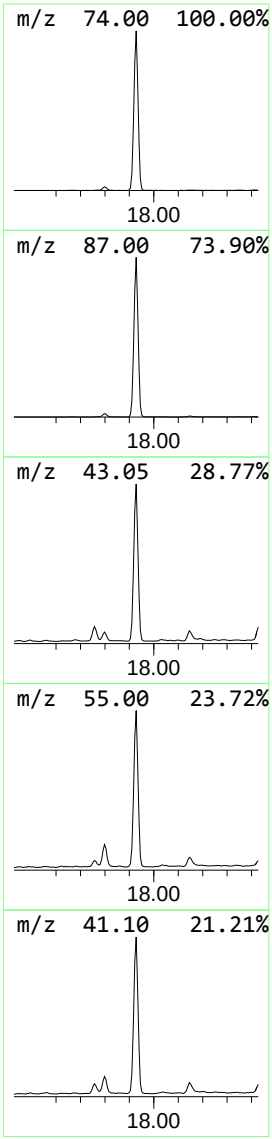
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.928	27.13 ng	7537890	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

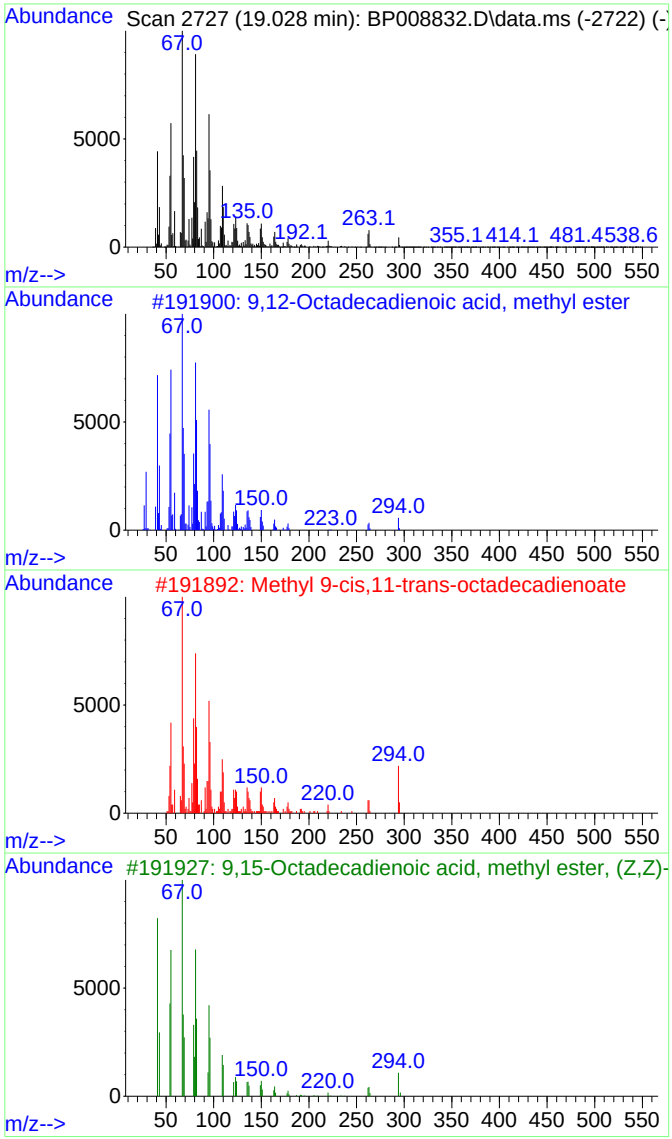
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

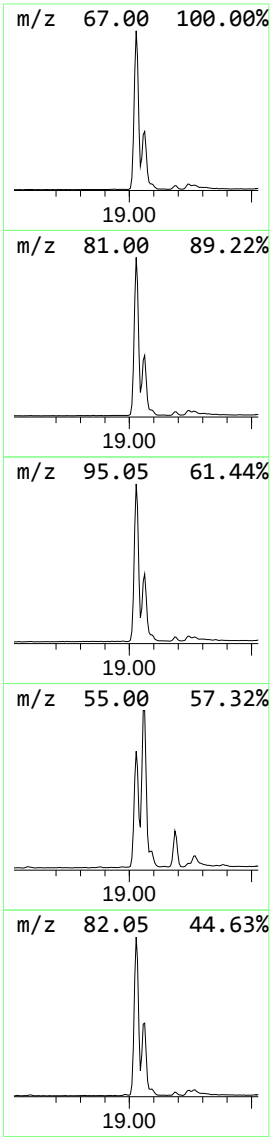
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.028	41.05 ng	11403500	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

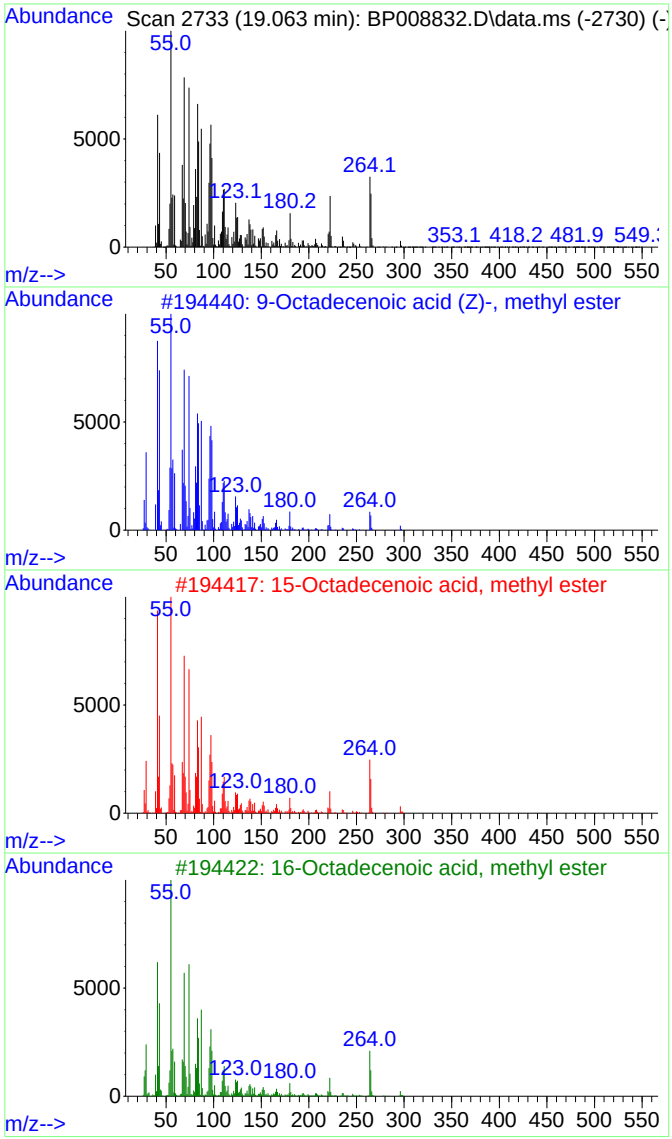
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

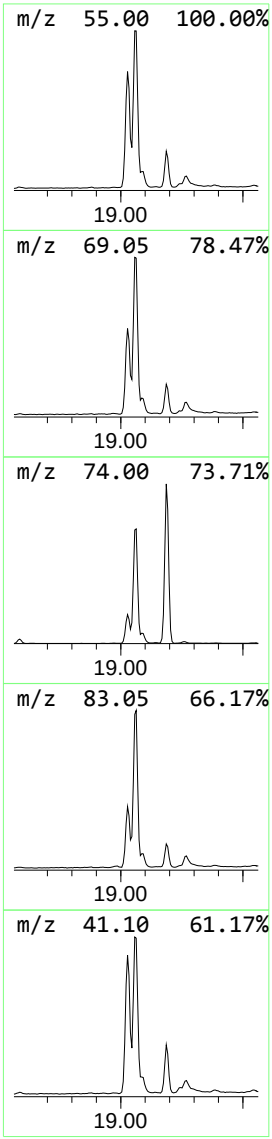
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.063	36.78 ng	10218300	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

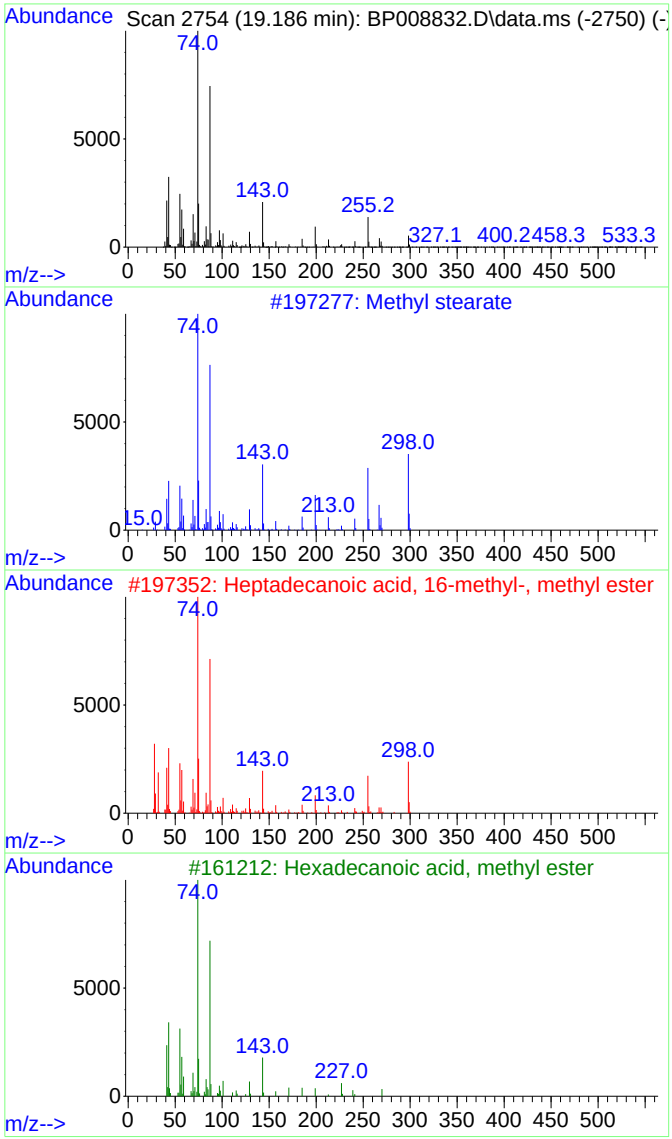
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

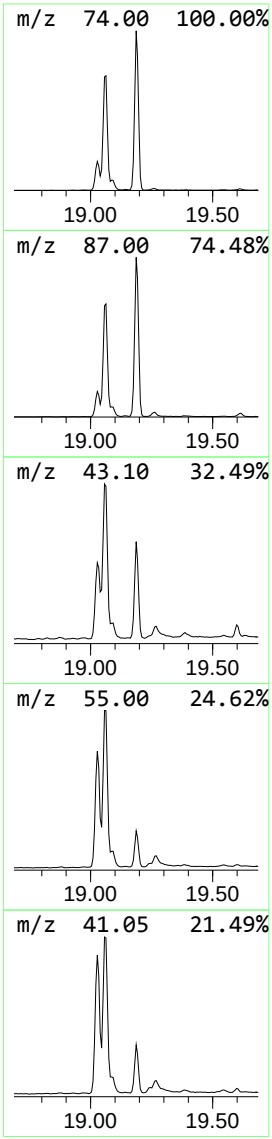
****

Peak Number 6 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	11.90 ng	3305320	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

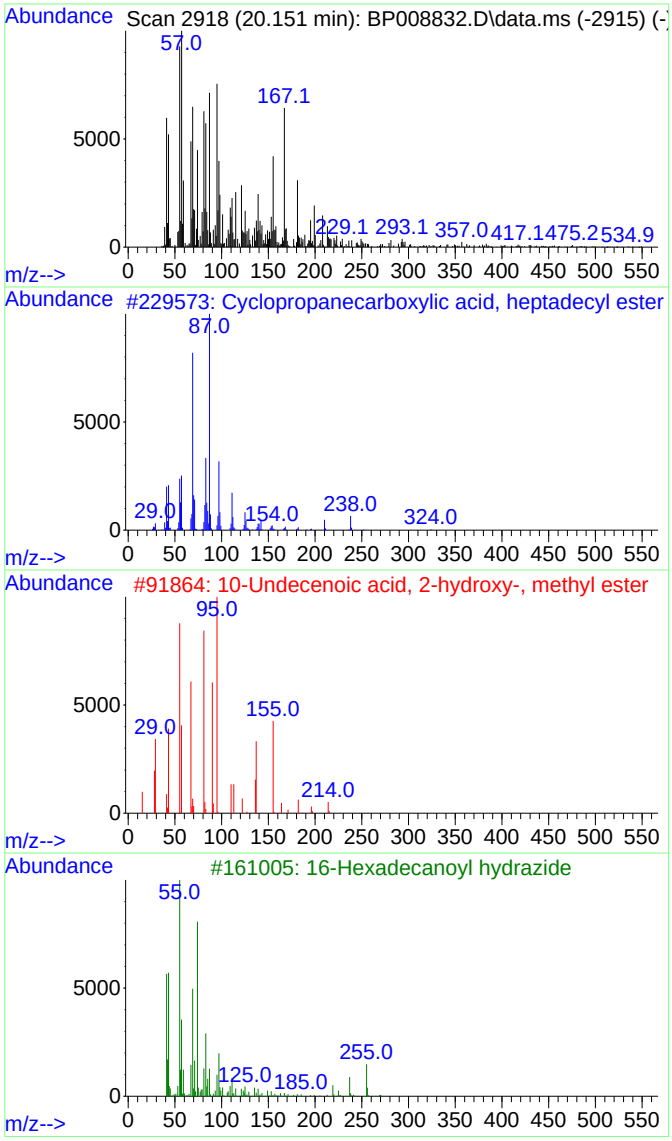
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

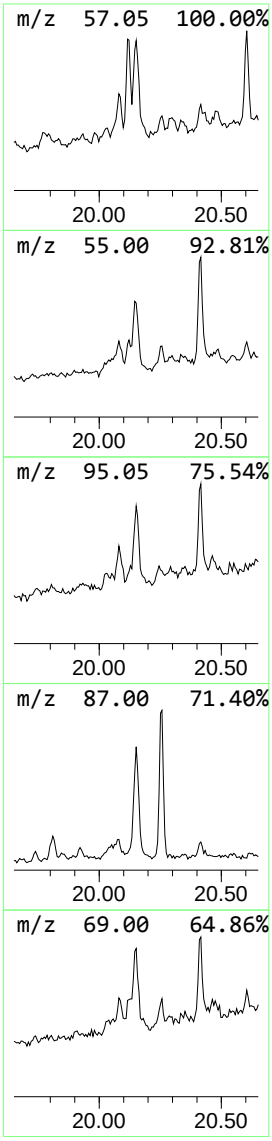
****

Peak Number 7 unknown20.151 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.151	2.09 ng	530399	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, hep...	324	C21H40O2	1000282-78-5	25
2	10-Undecenoic acid, 2-hydroxy-, ...	214	C12H22O3	055030-55-2	20
3	16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	18
4	2,6,6,10-Tetramethyl-undeca-8,10...	236	C15H24O2	098419-16-0	15
5	i-Propyl 11,12-methylene-octadec...	338	C22H42O2	1000336-77-0	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

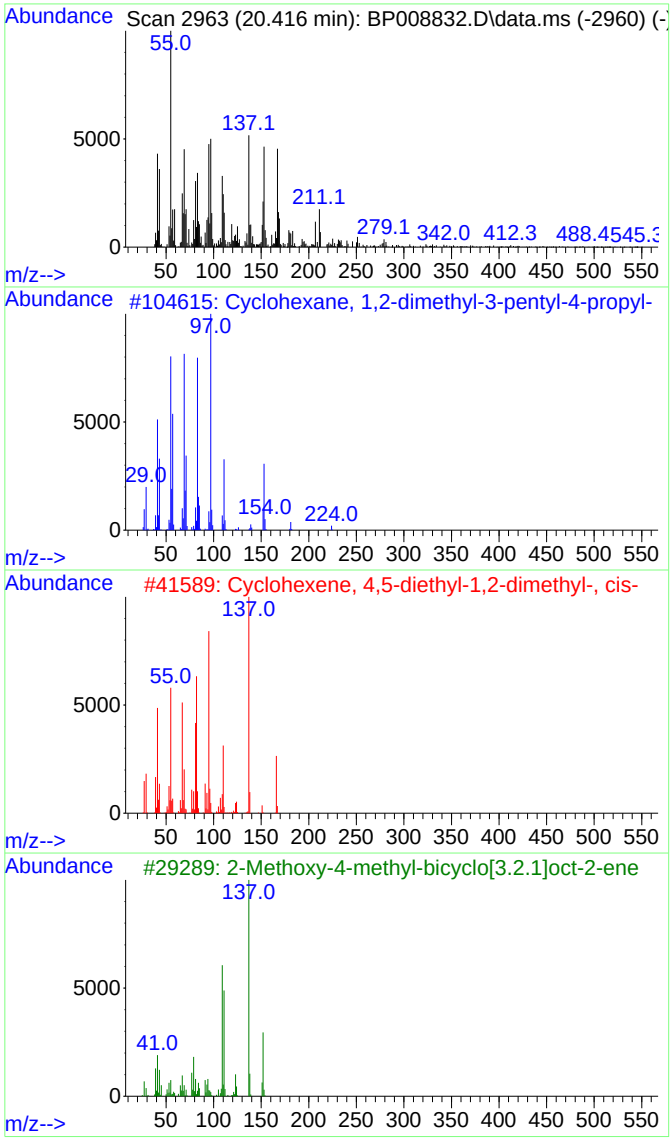
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

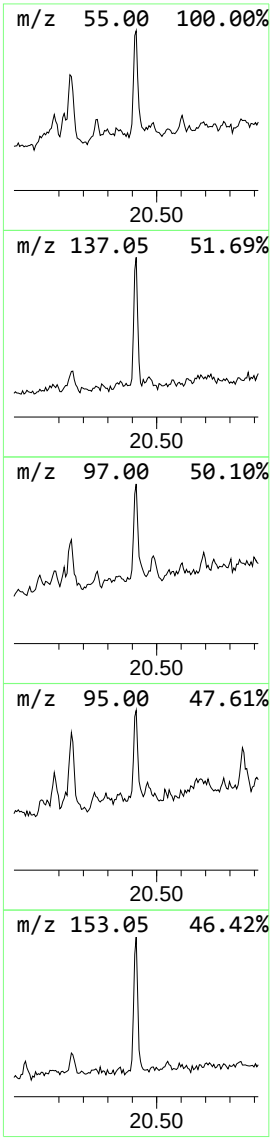
****

Peak Number 8 unknown20.416 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.416	2.09 ng	530809	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	25
2	Cyclohexene, 4,5-diethyl-1,2-dim...	166	C12H22	014113-70-3	22
3	2-Methoxy-4-methyl-bicyclo[3.2.1...	152	C10H16O	1000188-09-4	20
4	2-Ethyl-5-undecyl-.delta.1--pyrr...	251	C17H33N	114640-31-2	18
5	1(2H)-Naphthalenone, octahydro-,...	152	C10H16O	1000141-71-1	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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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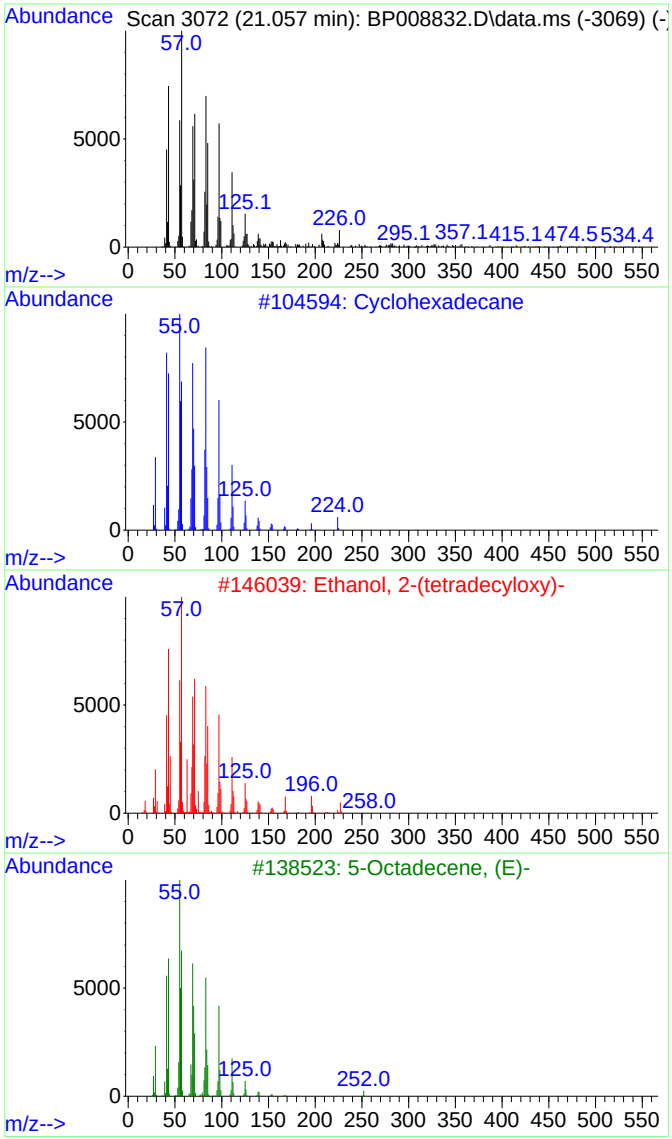
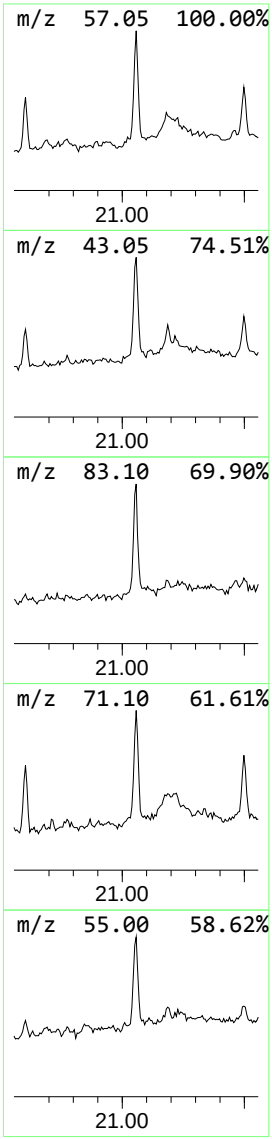
Peak Number 9 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	2.36 ng	600587	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	96
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	Cyclopentadecane	210	C15H30	000295-48-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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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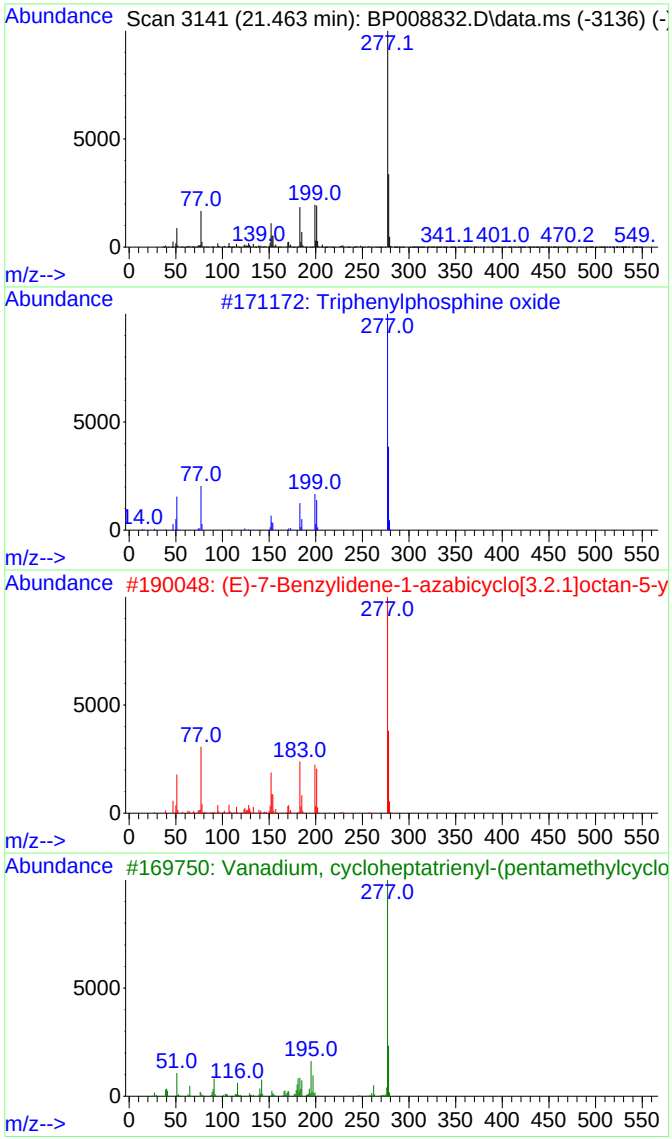
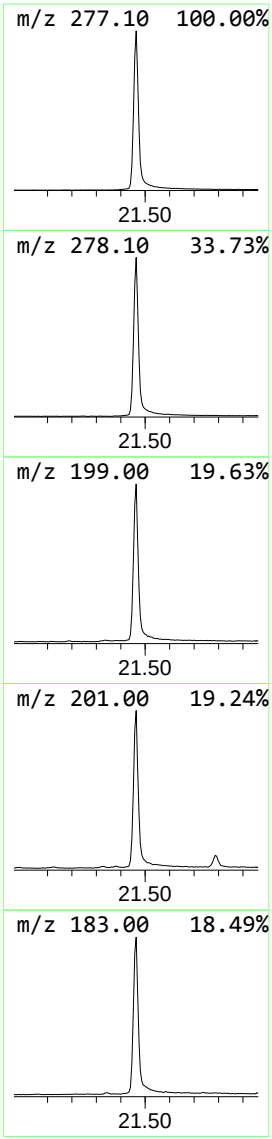
Peak Number 10 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.463	25.92 ng	6591100	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011722\
Data File : BP008832.D
Acq On : 17 Jan 2022 19:48
Operator : CG/JU
Sample : N1166-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SU-03-011422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP011422.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...	3.052	10.4	ng	1171440	1	7.852	2257630	20.0
9-Hexadecenoic ...	17.798	2.5	ng	700880	4	17.251	5556190	20.0
Hexadecanoic ac...	17.928	27.1	ng	7537890	4	17.251	5556190	20.0
9,12-Octadecadi...	19.028	41.0	ng	11403500	4	17.251	5556190	20.0
9-Octadecenoic ...	19.063	36.8	ng	10218300	4	17.251	5556190	20.0
Methyl stearate	19.186	11.9	ng	3305320	4	17.251	5556190	20.0
unknown20.151	20.151	2.1	ng	530399	5	21.345	5085240	20.0
unknown20.416	20.416	2.1	ng	530809	5	21.345	5085240	20.0
Cyclohexadecane	21.057	2.4	ng	600587	5	21.345	5085240	20.0
Triphenylphosph...	21.463	25.9	ng	6591100	5	21.345	5085240	20.0