LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
Acq On : 18 Dec 2021 15:08
Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

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_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126254.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	13	rVB	839267	1016313	18.38%	2.194%
2	2.240	21	26	31	rVB	99901	127860	2.31%	0.276%
3	3.281	200	203	208	rBV	48780	80131	1.45%	0.173%
4	4.410	391	395	399	rVB	51053	61436	1.11%	0.133%
5	5.034	491	501	513	rBV	1156432	1513892	27.39%	3.268%
6	5.434	563	569	572	rBV	4777493	5392828	97.55%	11.641%
7	5.828	633	636	640	rVB	179294	157538	2.85%	0.340%
8	6.445	734	741	744	rBV	4312402	5528065	100.00%	11.933%
9	6.816	800	804	807	rBV	1583425	1265935	22.90%	2.733%
10	7.375	893	899	903	rBV	3192684	3752541	67.88%	8.100%
11	8.004	1002	1006	1017	rBV	34039	56749	1.03%	0.123%
12	8.098	1017	1022	1025	rBV	2048238	1793298	32.44%	3.871%
13	9.175	1200	1205	1209	rBV	4853615	5472518	99.00%	11.813%
14	9.263	1216	1220	1223	rBV2	101475	85842	1.55%	0.185%
15	9.292	1223	1225	1229	rVB	77964	72039	1.30%	0.156%
16	9.675	1286	1290	1298	rBV6	31254	68309	1.24%	0.147%
17	9.851	1313	1320	1324	rBV	2180310	1932219	34.95%	4.171%
18	10.269	1387	1391	1393	rBV2	76175	76186	1.38%	0.164%
19	10.639	1448	1454	1458	rBV	3258584	3409597	61.68%	7.360%
20	11.304	1562	1567	1569	rBV2	105351	100851	1.82%	0.218%
21	11.333	1569	1572	1576	rVV	2035951	1909845	34.55%	4.123%
22	11.404	1578	1584	1587	rBV3	122842	146302	2.65%	0.316%
23	11.598	1612	1617	1622	rBV6	48003	109311	1.98%	0.236%
24	11.739	1637	1641	1644	rVB	787643	633476	11.46%	1.367%
25	11.868	1660	1663	1667	rBV	334335	291322	5.27%	0.629%
26	12.445	1754	1761	1764	rBV	999403	943079	17.06%	2.036%
27	12.527	1771	1775	1780	rVB	165471	154019	2.79%	0.332%
28	12.592	1780	1786	1789	rVB2	96510	118224	2.14%	0.255%
29	12.651	1793	1796	1799	rBV	68477	64928	1.17%	0.140%
30	12.927	1838	1843	1846	rBV	4743273	5121626	92.65%	11.056%
31	13.857	1994	2001	2016	rBV	292245	756209	13.68%	1.632%
32	13.968	2016	2020	2024	rVV2	1721623	1752854	31.71%	3.784%
33	14.068	2031	2037	2043	rBV	210459	246561	4.46%	0.532%
34	14.733	2146	2150	2152	rBV	98317	101937	1.84%	0.220%
35	14.833	2163	2167	2170	rVB	152651	149932	2.71%	0.324%
36	15.092	2208	2211	2217	rVB	63027	71603	1.30%	0.155%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
Acq On : 18 Dec 2021 15:08
Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

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_F\Methods\8270-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.415	2261	2266	2271	rBV2	1046921	1325982	23.99%	2.862%
38	15.462	2271	2274	2280	rVB	74404	106137	1.92%	0.229%
39	15.898	2343	2348	2352	rBV	65178	96033	1.74%	0.207%
40	16.015	2363	2368	2383	rBV	27206	95479	1.73%	0.206%
41	16.392	2428	2432	2442	rVB	54912	106020	1.92%	0.229%
42	16.980	2527	2532	2538	rVB2	29962	60668	1.10%	0.131%

Sum of corrected areas: 46325694

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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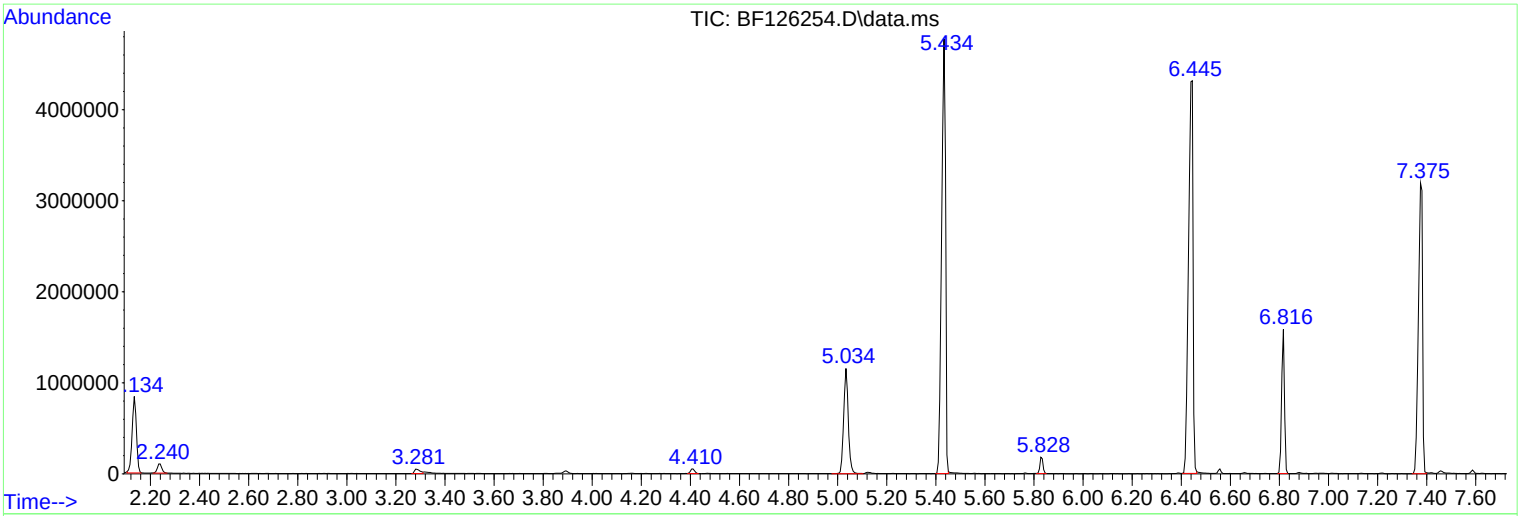
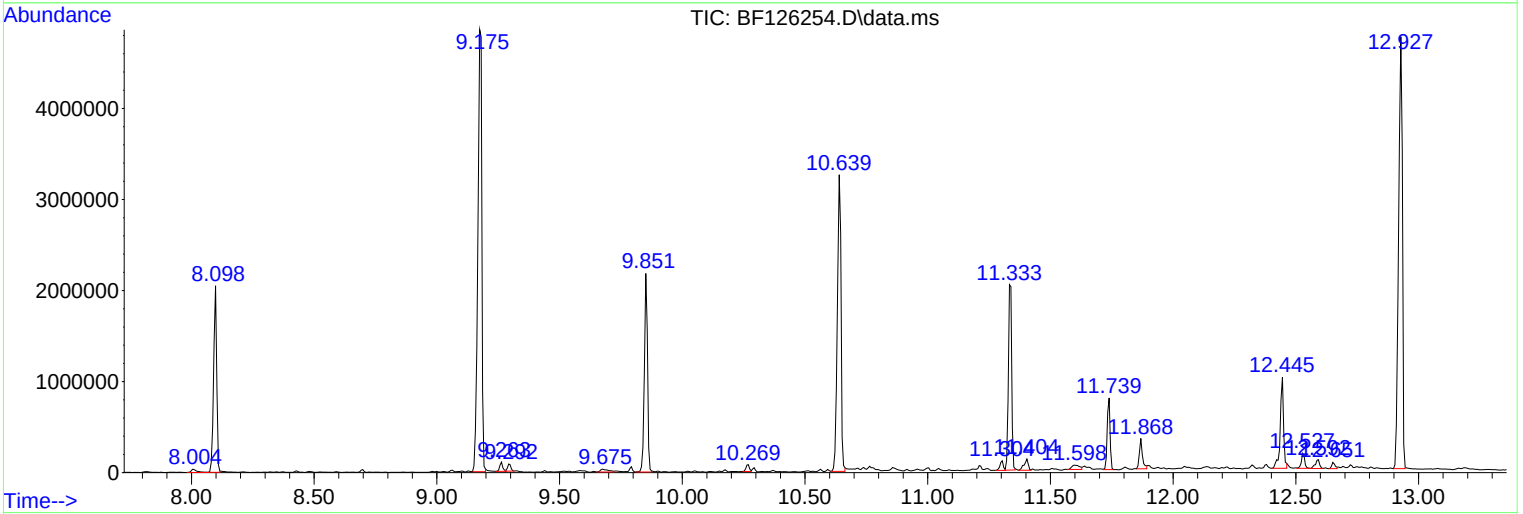
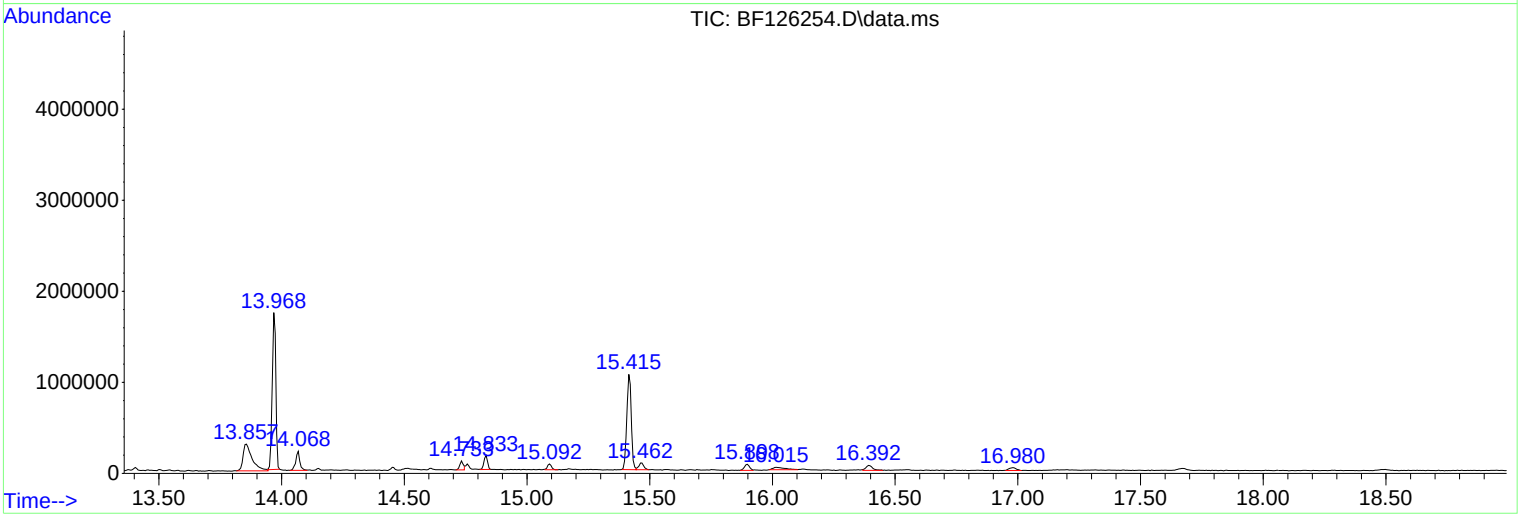
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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_F\Data\BF121821\
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Operator : JU/CG
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

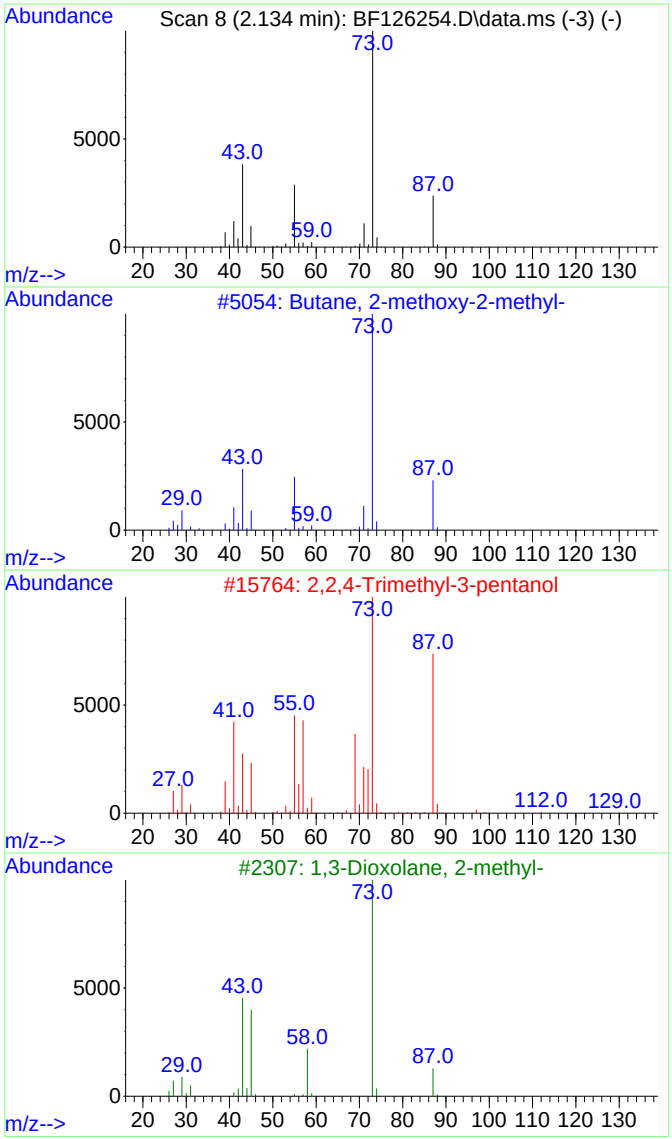
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

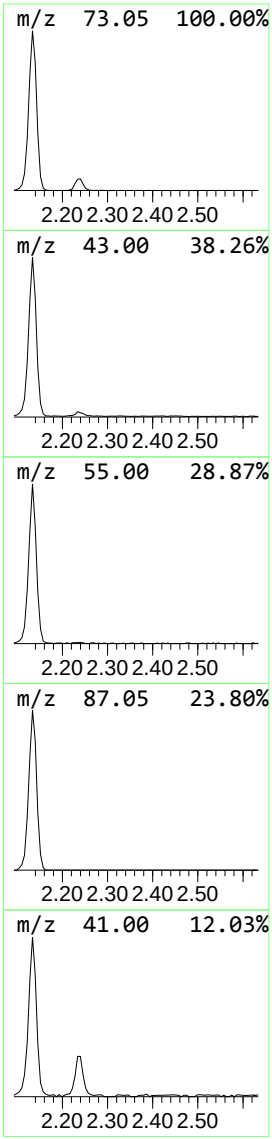
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	16.06 ng	1016310	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

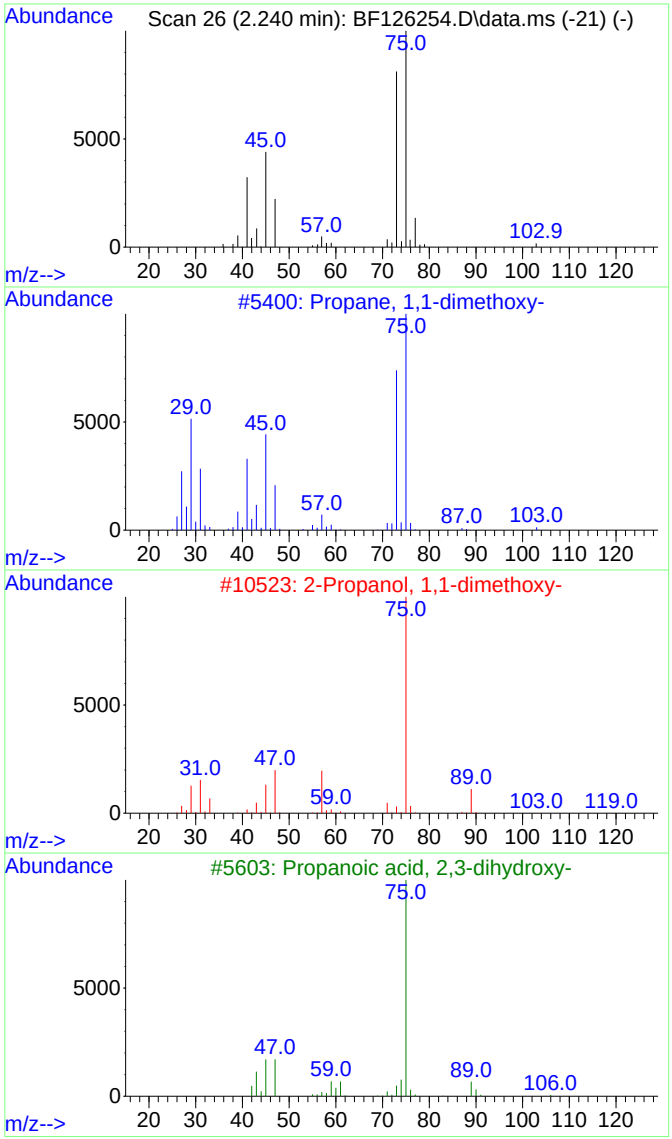
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

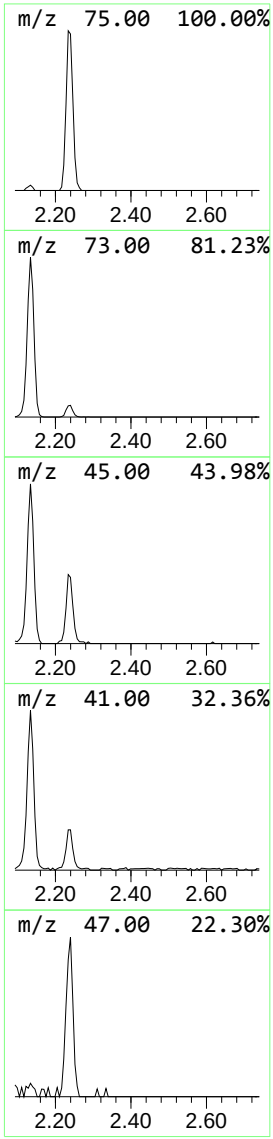
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	2.02 ng	127860	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
3	Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	33
4	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	28
5	Pentanoic acid, 2-hydroxy-, ethy...	146	C7H14O3	006938-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
Acq On : 18 Dec 2021 15:08
Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

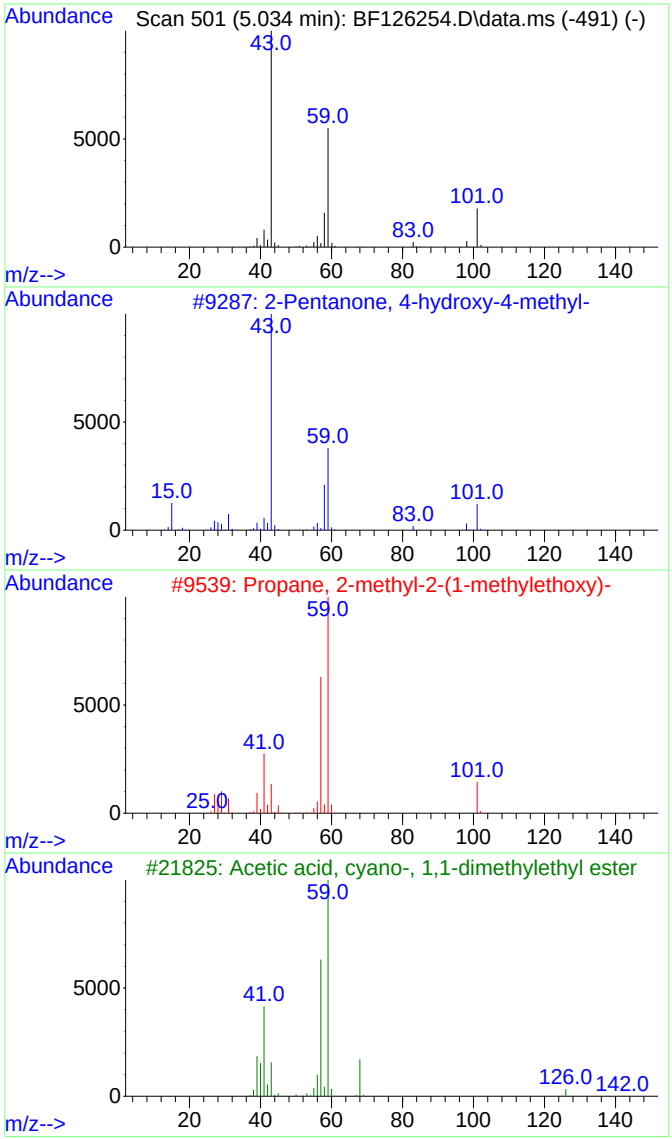
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

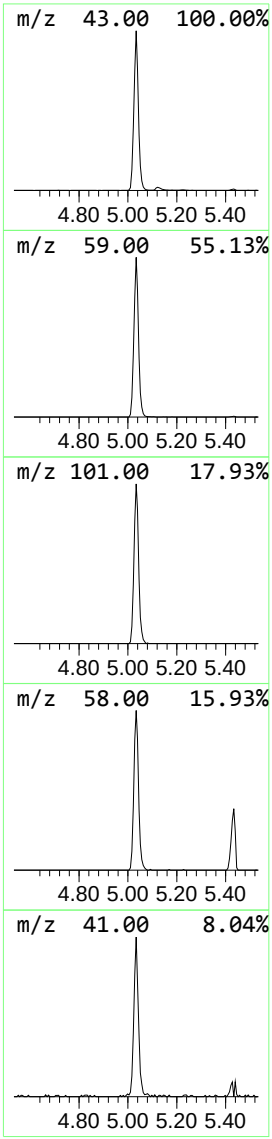
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	23.92 ng	1513890	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
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Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

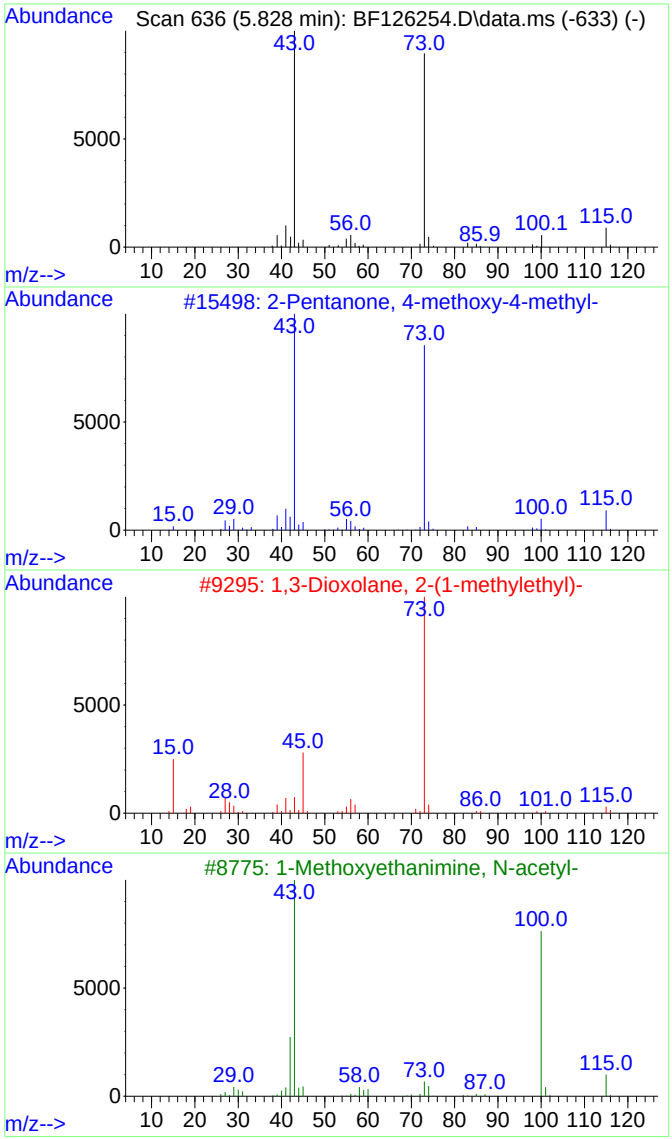
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

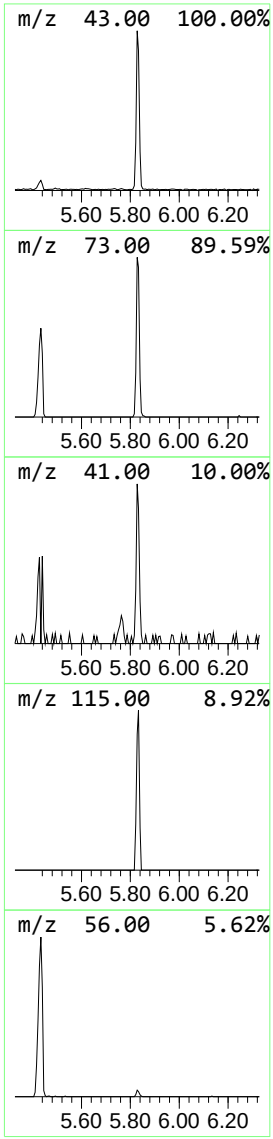
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.49 ng	157538	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
4	3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	12
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10





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Data File : BF126254.D
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Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

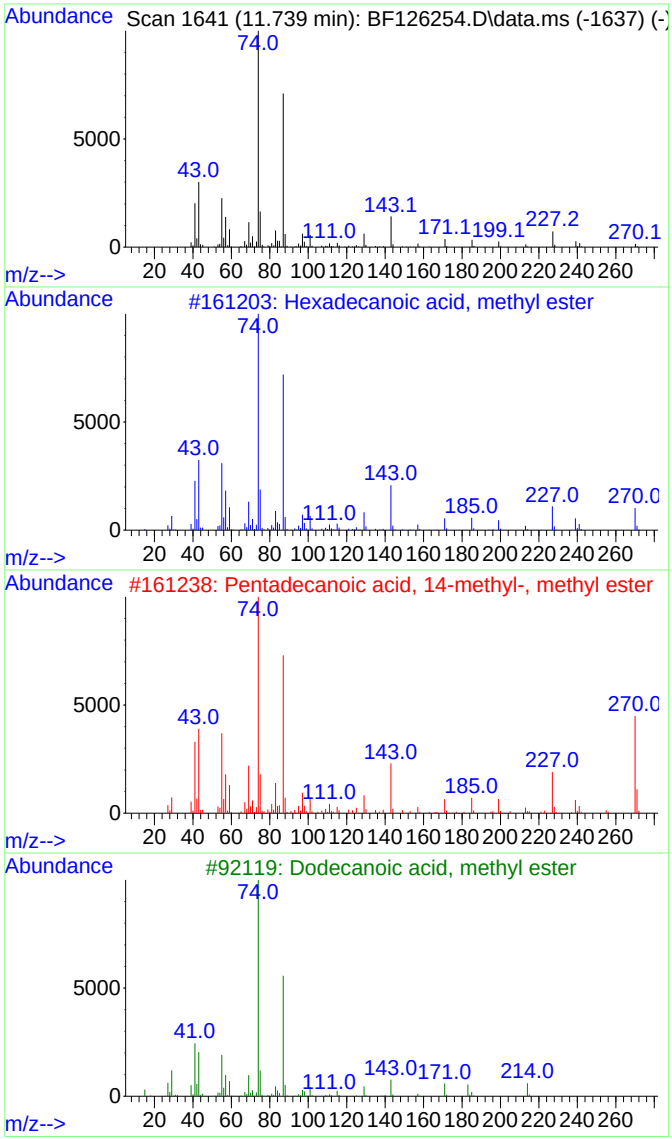
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

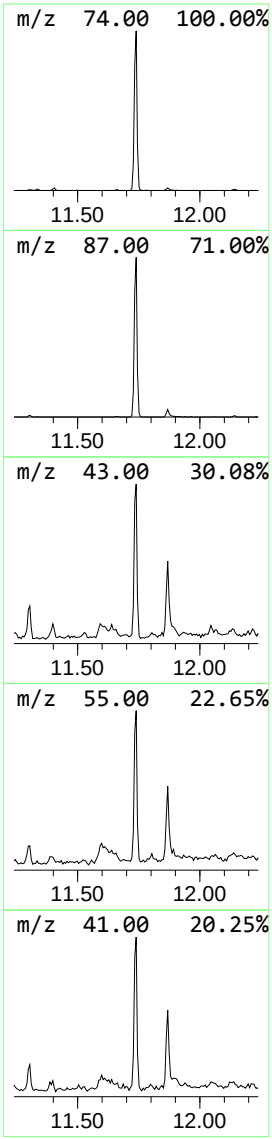
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	6.63 ng	633476	Phenanthrene-d10	11.339

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	94
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

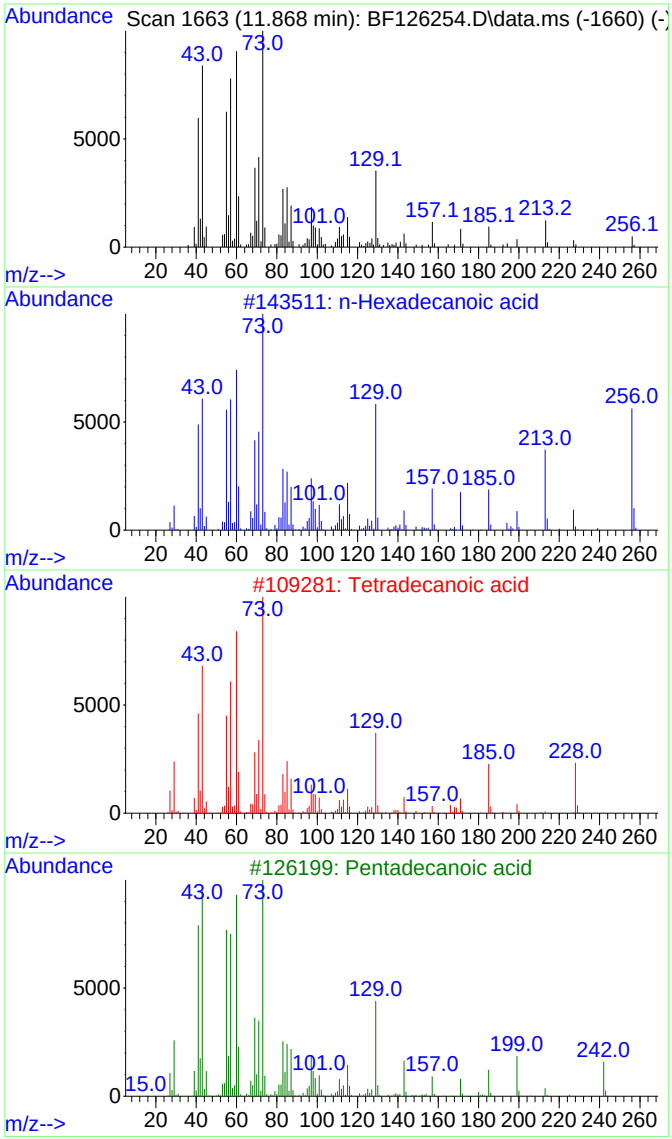
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

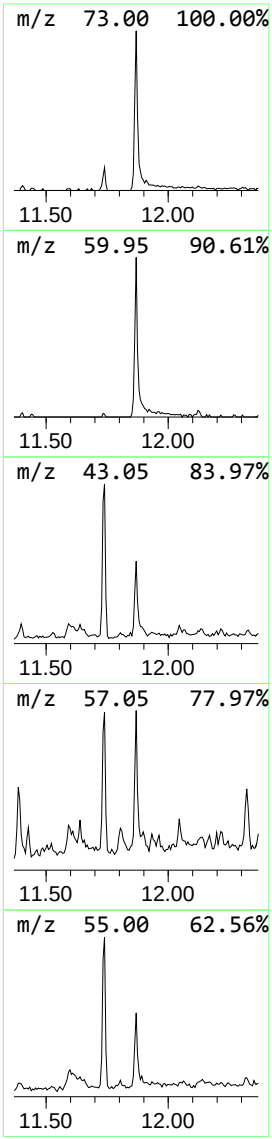
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.868	3.05 ng	291322	Phenanthrene-d10	11.339

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	15





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

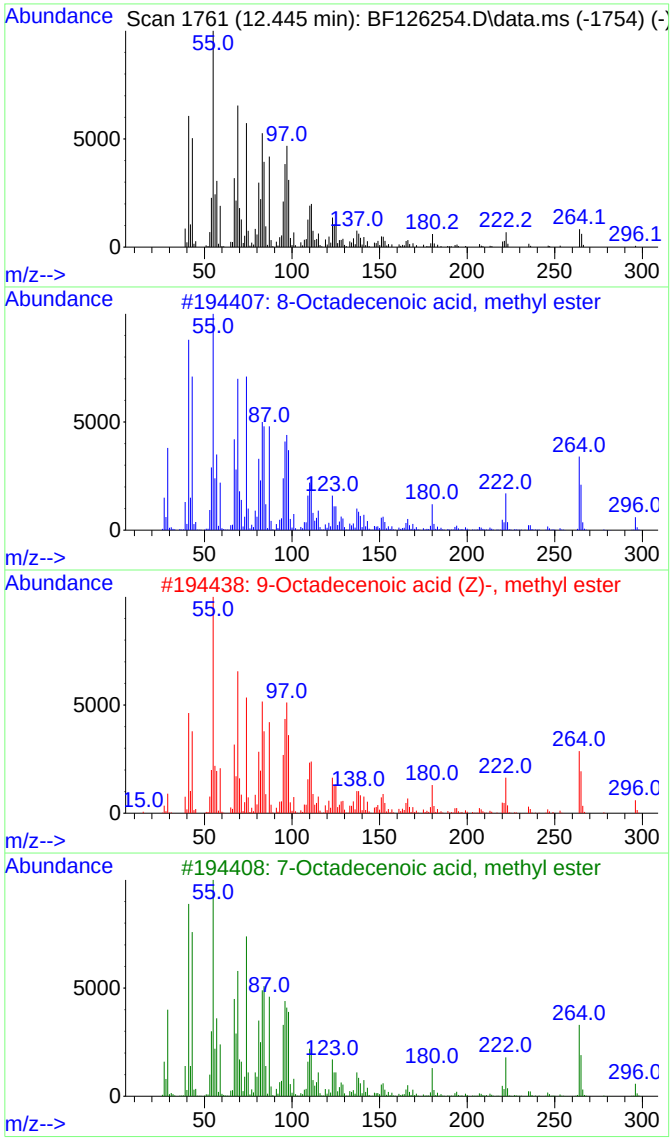
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

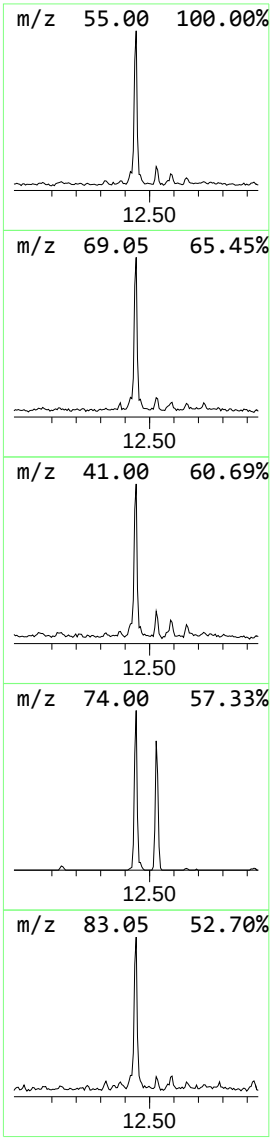
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 8-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	9.88 ng	943079	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	97
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
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Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

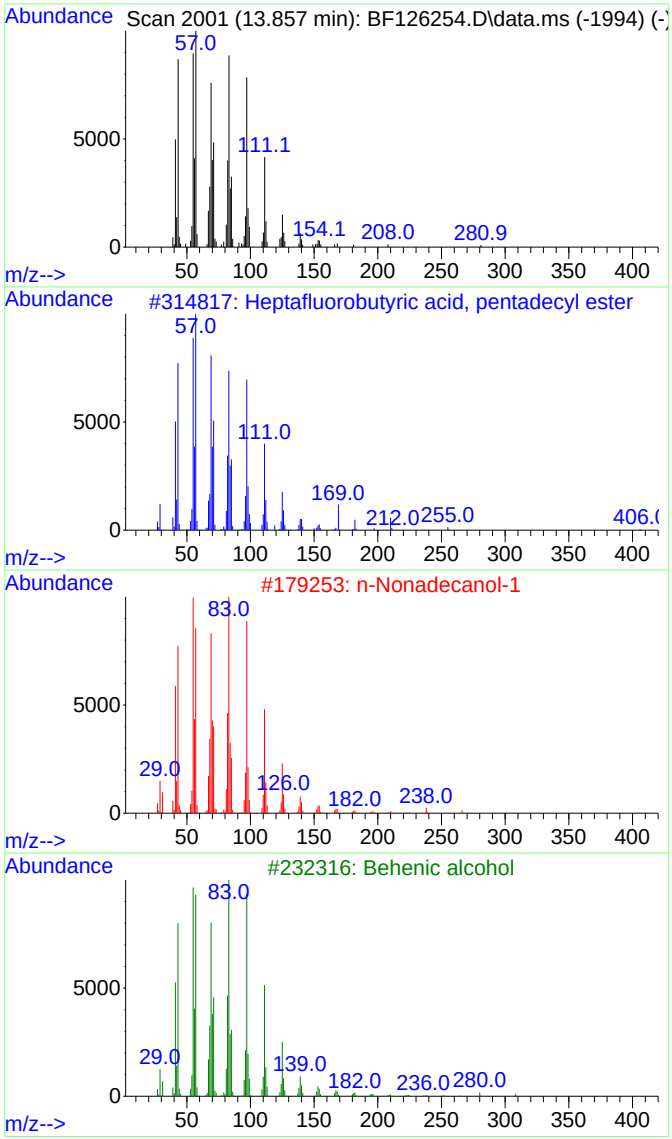
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

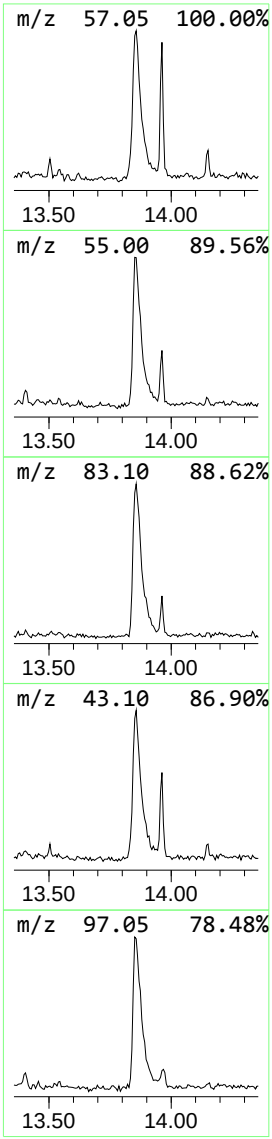
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	8.63 ng	756209	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
Acq On : 18 Dec 2021 15:08
Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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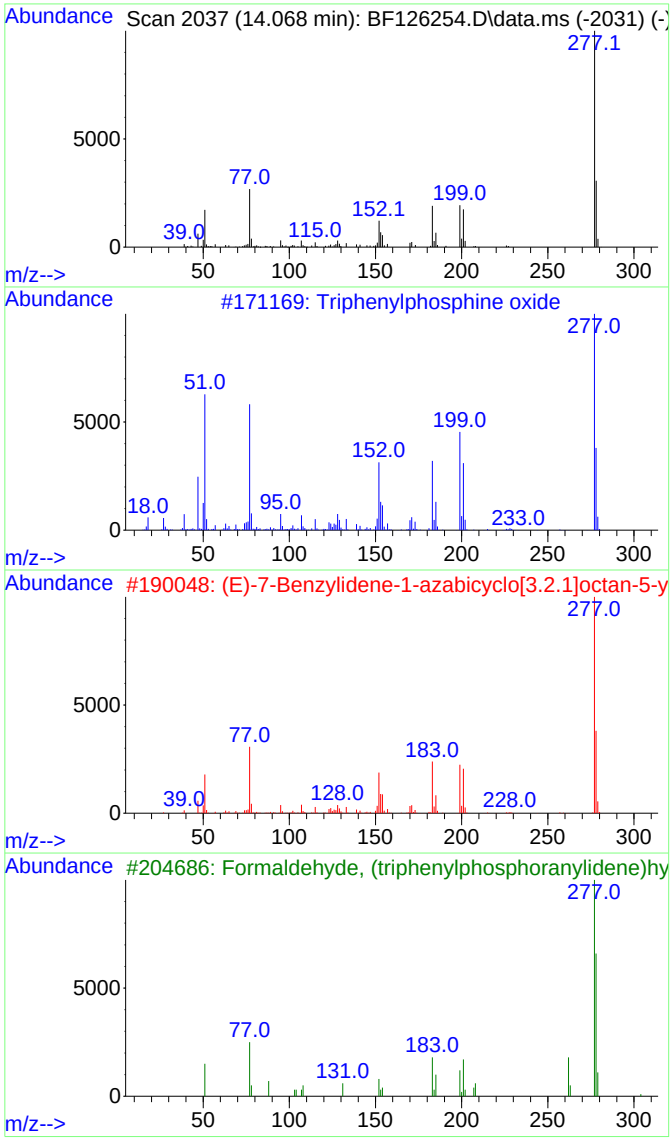
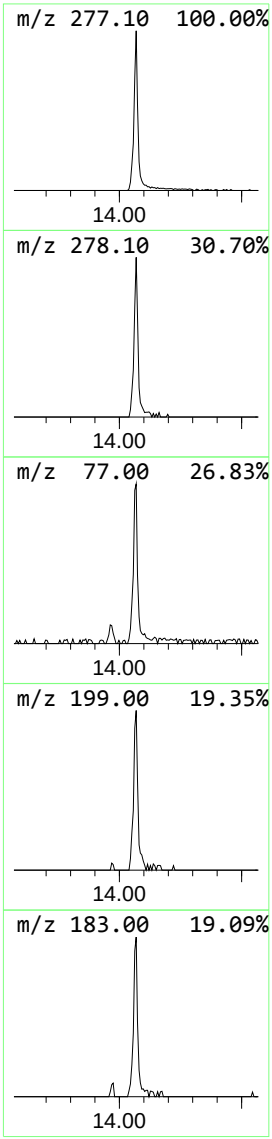
Peak Number 9 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	2.81 ng	246561	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	76
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
Acq On : 18 Dec 2021 15:08
Operator : JU/CG
Sample : M5082-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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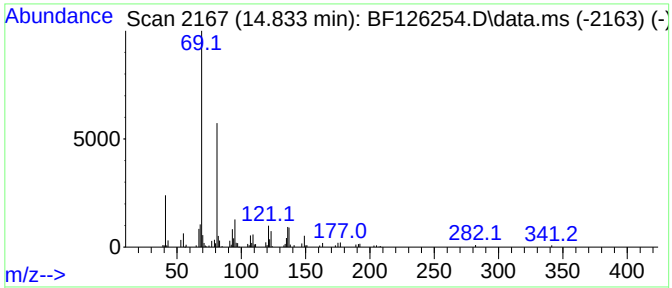
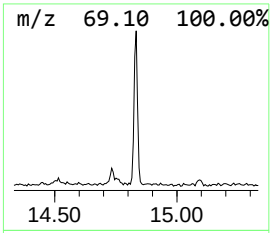
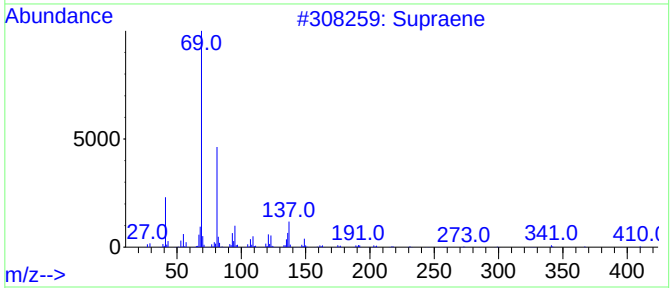
Peak Number 10 Supraene Concentration Rank 9

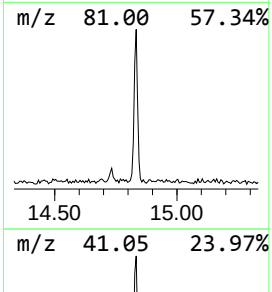
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.26 ng	149932	Perylene-d12	15.415

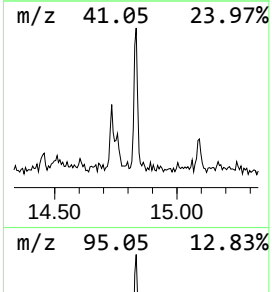
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72

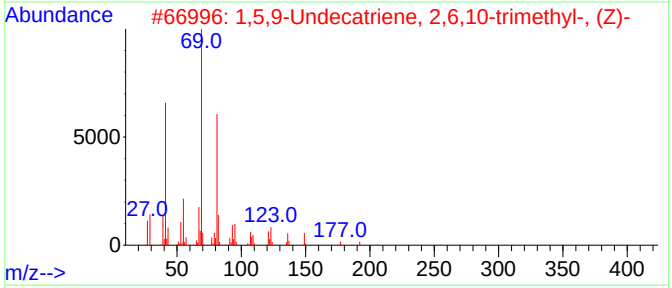


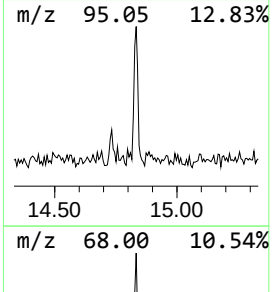


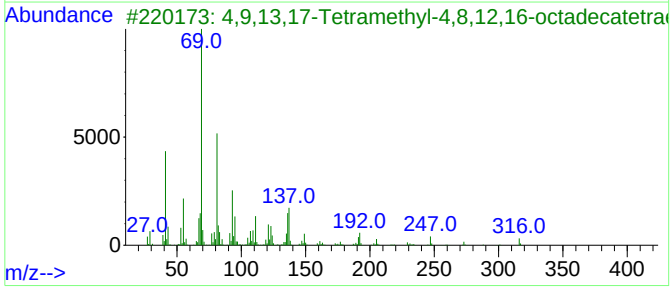


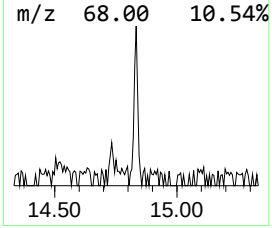












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126254.D
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BNA_F
ClientSampleId :
SASP2-121-1(65-77.7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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...	2.134	16.1	ng	1016310	1	6.816	1265940	20.0
Propane, 1,1-di...	2.240	2.0	ng	127860	1	6.816	1265940	20.0
2-Pentanone, 4-...	5.034	23.9	ng	1513890	1	6.816	1265940	20.0
2-Pentanone, 4-...	5.828	2.5	ng	157538	1	6.816	1265940	20.0
Hexadecanoic ac...	11.739	6.6	ng	633476	4	11.339	1909850	20.0
n-Hexadecanoic ...	11.868	3.0	ng	291322	4	11.339	1909850	20.0
8-Octadecenoic ...	12.445	9.9	ng	943079	4	11.339	1909850	20.0
Heptafluorobuty...	13.857	8.6	ng	756209	5	13.968	1752850	20.0
Triphenylphosph...	14.068	2.8	ng	246561	5	13.968	1752850	20.0
Supraene	14.833	2.3	ng	149932	6	15.415	1325980	20.0