LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126648.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.305	29	37	43	rVB	1422623	1897692	57.49%	7.545%
2	3.534	242	246	254	rBV	33155	55366	1.68%	0.220%
3	5.199	526	529	538	rVB	108552	128319	3.89%	0.510%
4	5.581	589	594	597	rBV	3095143	2900778	87.88%	11.534%
5	6.087	676	680	682	rBV	85704	83812	2.54%	0.333%
6	6.110	682	684	692	rVB	122391	127173	3.85%	0.506%
7	6.575	757	763	766	rBV	2982290	3070641	93.03%	12.209%
8	6.963	825	829	832	rBV	878053	713177	21.61%	2.836%
9	7.522	919	924	927	rBV	2173006	2058827	62.37%	8.186%
10	8.245	1043	1047	1050	rBV	1054914	911189	27.61%	3.623%
11	9.322	1225	1230	1233	rBV	3723475	3300811	100.00%	13.124%
12	9.392	1239	1242	1245	rBV	81870	60271	1.83%	0.240%
13	9.798	1308	1311	1316	rVB4	25195	38445	1.16%	0.153%
14	9.922	1327	1332	1335	rVB	42771	37011	1.12%	0.147%
15	10.004	1341	1346	1349	rBV	1234800	1018859	30.87%	4.051%
16	10.792	1476	1480	1483	rBV	1996432	1702793	51.59%	6.770%
17	10.898	1496	1498	1504	rVB	33363	43180	1.31%	0.172%
18	11.492	1596	1599	1602	rBV	1108164	980238	29.70%	3.897%
19	11.516	1602	1603	1607	rVB	70773	52348	1.59%	0.208%
20	11.880	1662	1665	1668	rVB	122967	97181	2.94%	0.386%
21	12.004	1683	1686	1688	rBV2	39860	37110	1.12%	0.148%
22	12.569	1779	1782	1784	rBV2	137558	115504	3.50%	0.459%
23	12.586	1784	1785	1791	rVB2	131980	111709	3.38%	0.444%
24	12.675	1797	1800	1803	rBV	48982	38491	1.17%	0.153%
25	12.710	1803	1806	1815	rVB	136678	123876	3.75%	0.493%
26	12.939	1843	1845	1849	rVB	128048	107000	3.24%	0.425%
27	13.086	1865	1870	1873	rBV	3318244	2902820	87.94%	11.542%
28	13.974	2017	2021	2029	rBV2	234520	284183	8.61%	1.130%
29	14.116	2041	2045	2046	rBV	129006	103313	3.13%	0.411%
30	14.139	2046	2049	2052	rVV	760503	717829	21.75%	2.854%
31	14.163	2052	2053	2058	rVB	46944	39284	1.19%	0.156%
32	14.239	2058	2066	2069	rBV6	39432	77609	2.35%	0.309%
33	14.616	2125	2130	2133	rBV3	50568	74657	2.26%	0.297%
34	14.774	2154	2157	2162	rBV4	22183	38117	1.15%	0.152%
35	15.204	2227	2230	2234	rBV2	39492	61275	1.86%	0.244%
36	15.286	2240	2244	2247	rBV2	33273	39540	1.20%	0.157%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.321	2247	2250	2257	rVB6	21965	38817	1.18%	0.154%
38	15.527	2281	2285	2292	rVB	29995	41364	1.25%	0.164%
39	15.592	2292	2296	2301	rVB	36346	44617	1.35%	0.177%
40	15.663	2303	2308	2313	rBV	486804	641014	19.42%	2.549%
41	16.215	2397	2402	2411	rBV9	26611	61906	1.88%	0.246%
42	17.862	2674	2682	2691	rBV6	28154	69926	2.12%	0.278%
43	18.368	2761	2768	2778	rVB9	18280	49674	1.50%	0.198%
44	18.733	2823	2830	2839	rBV9	17851	52814	1.60%	0.210%

Sum of corrected areas: 25150560

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
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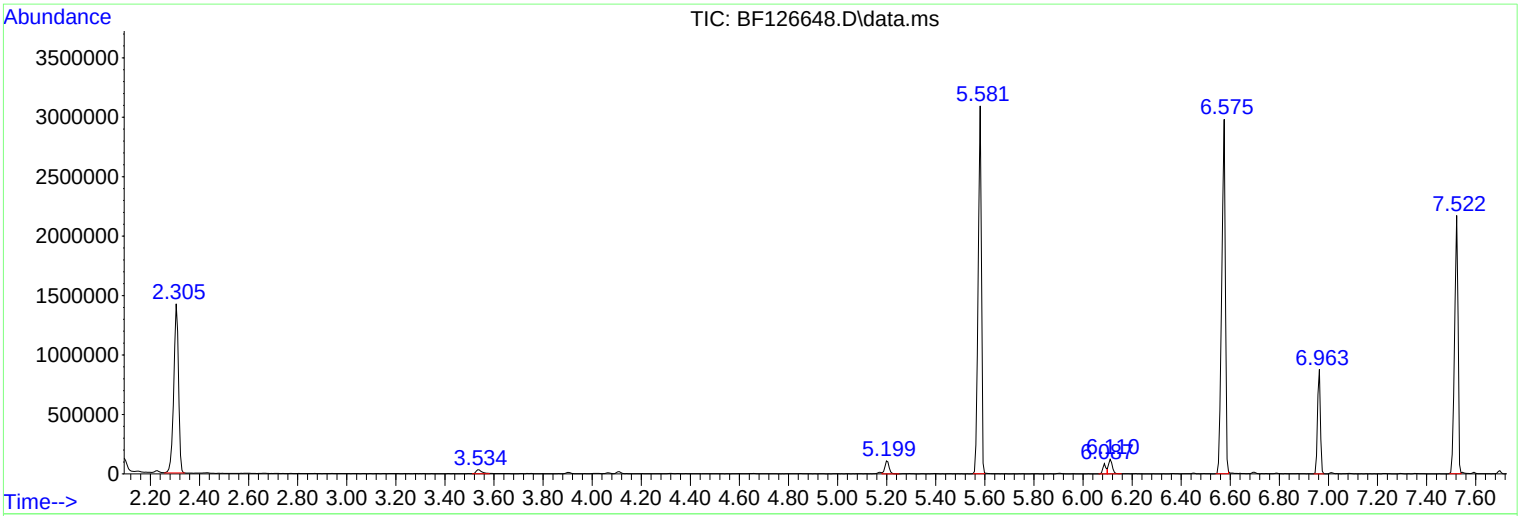
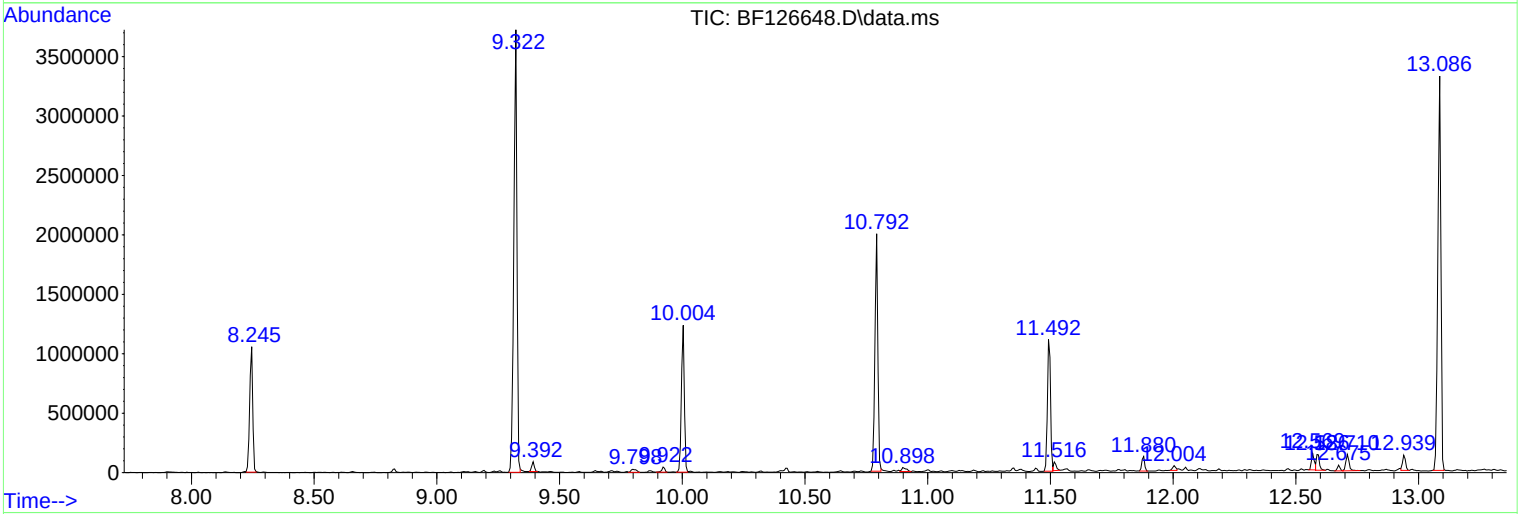
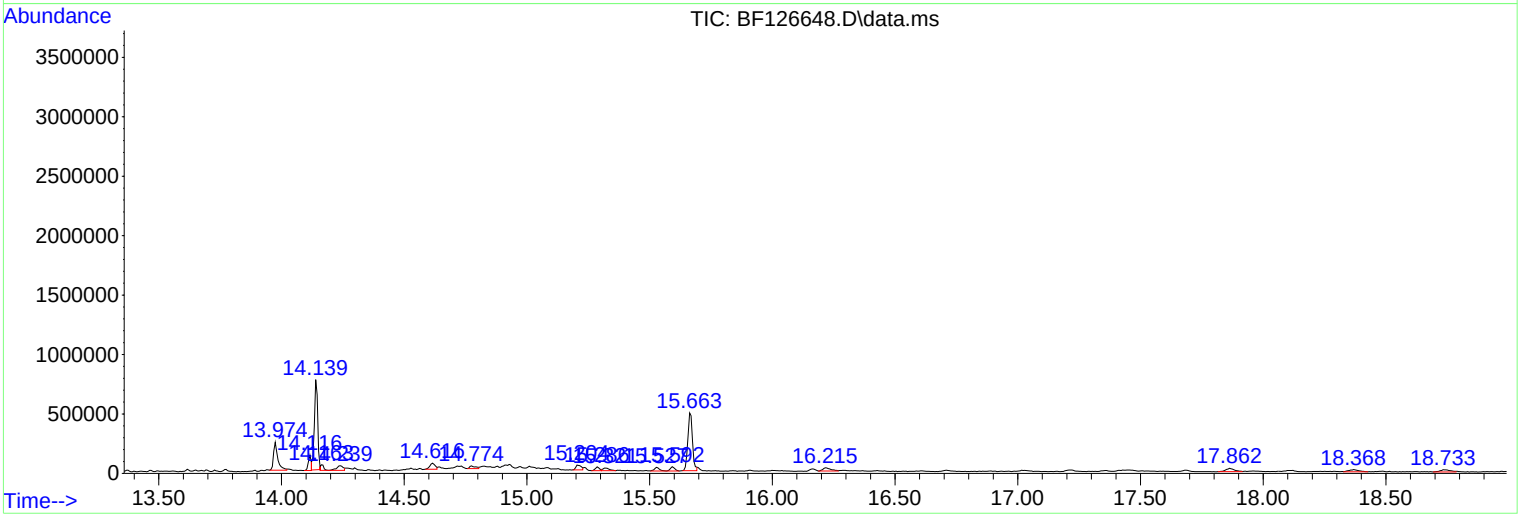
Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

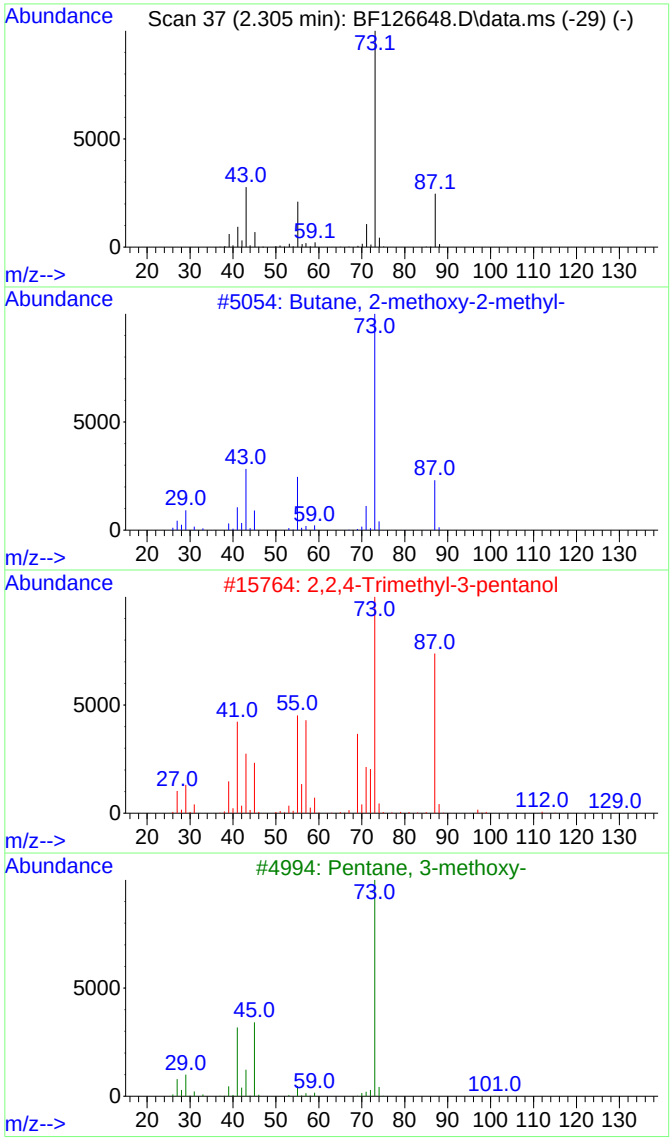
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

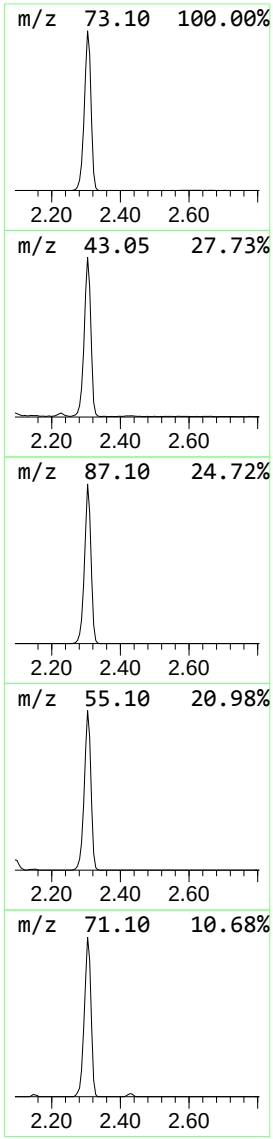
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	53.22 ng	1897690	1,4-Dichlorobenzene-d4	6.963

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
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Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

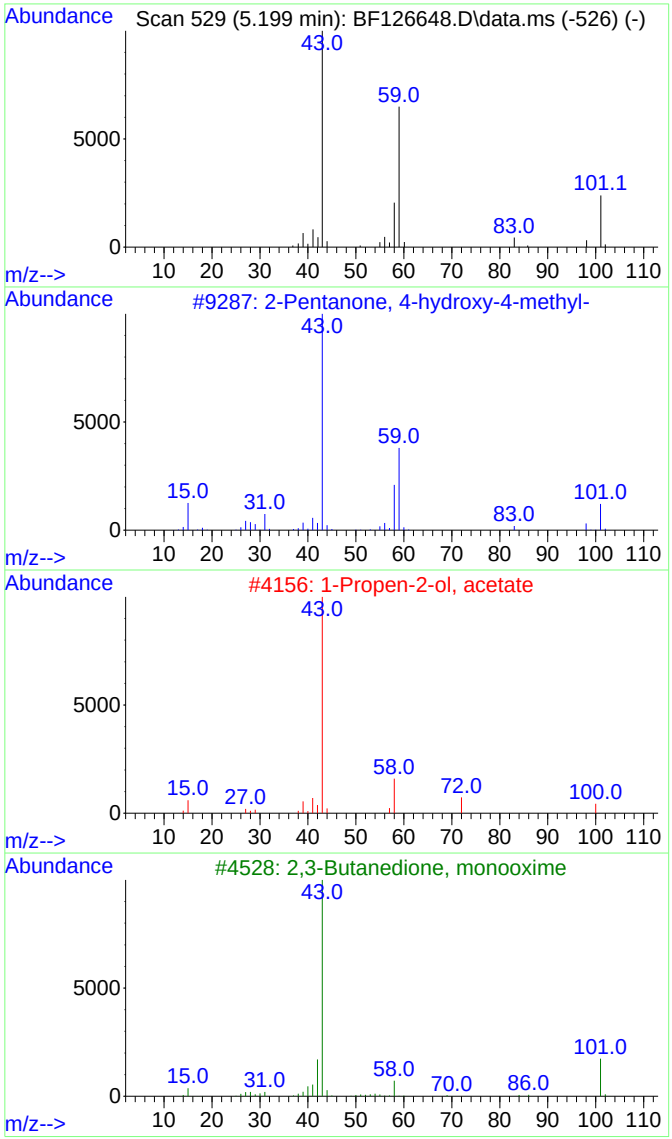
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

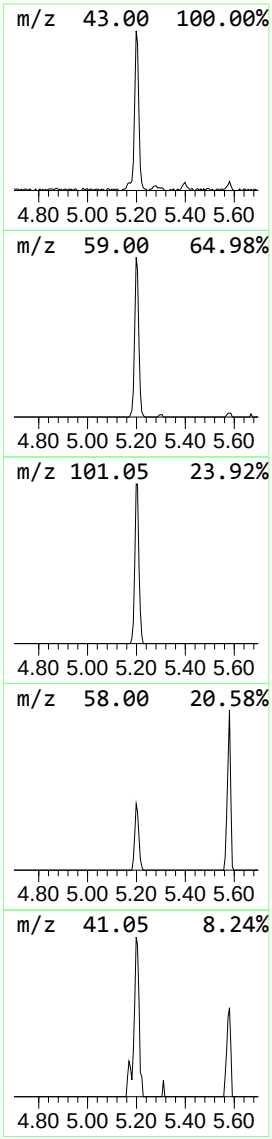
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	3.60 ng	128319	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

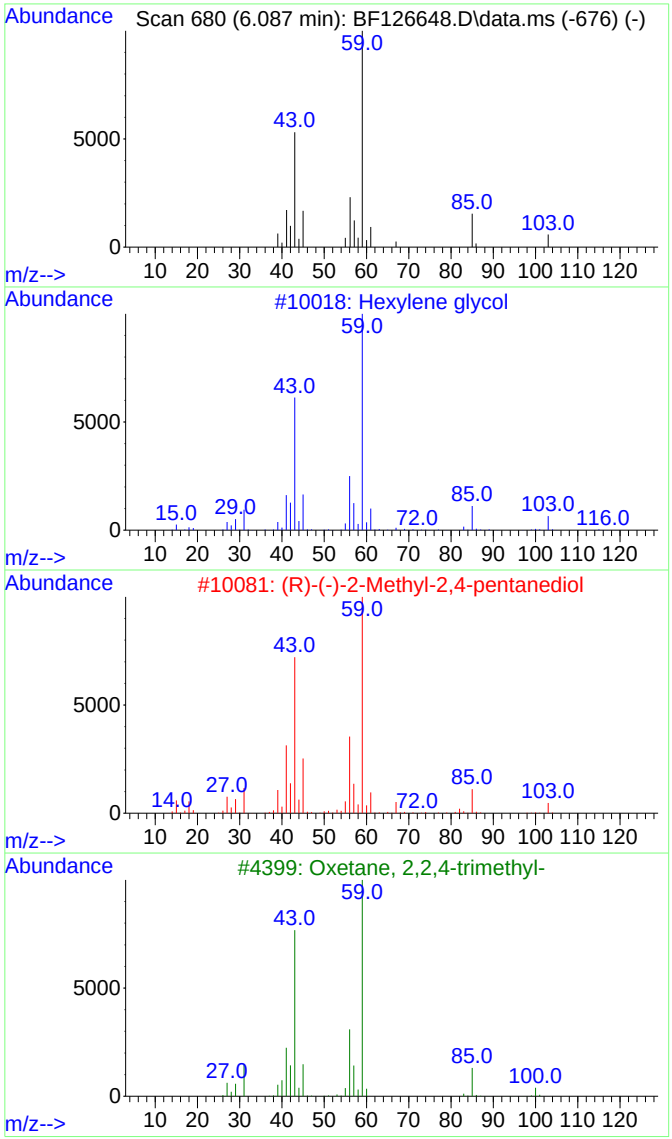
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

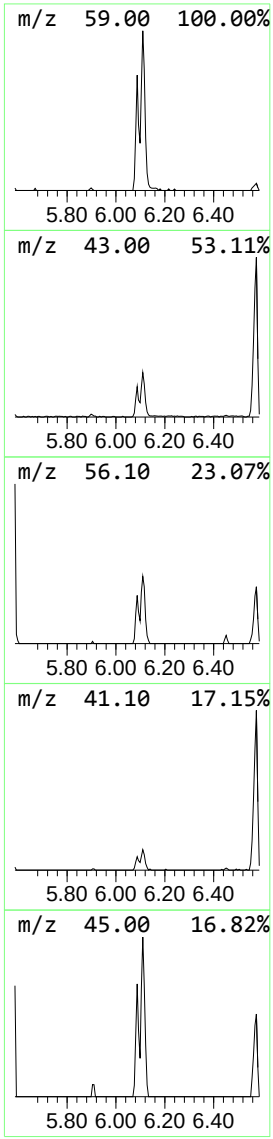
****

Peak Number 3 Hexylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.087	2.35 ng	83812	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	90
2	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	83
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	78
4	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	50
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
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Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

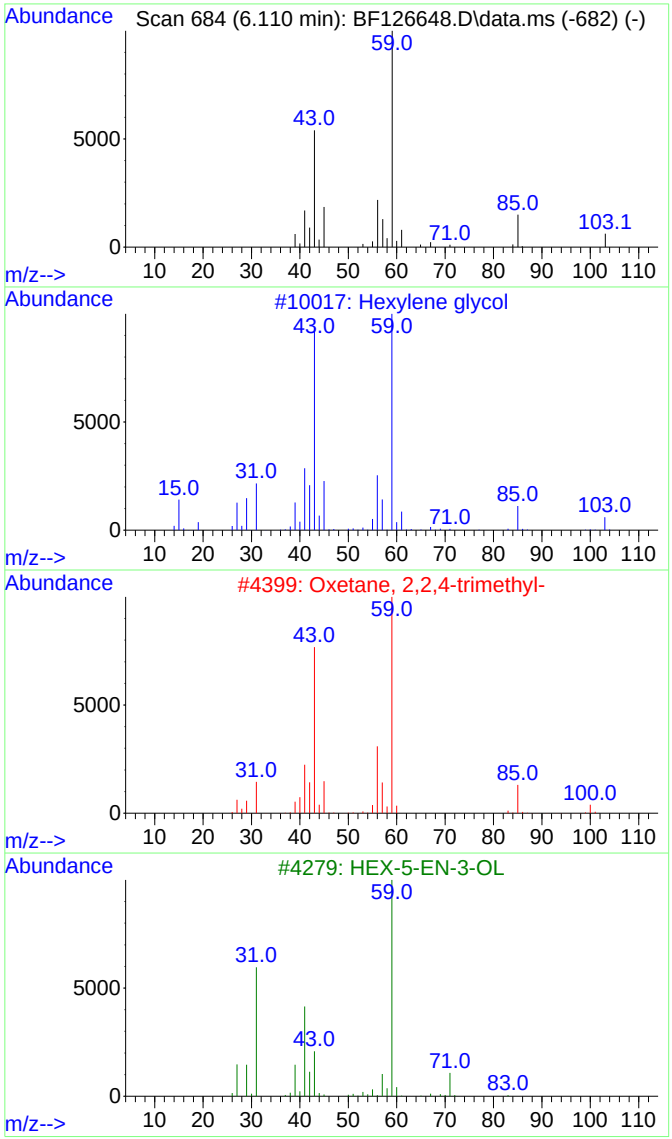
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

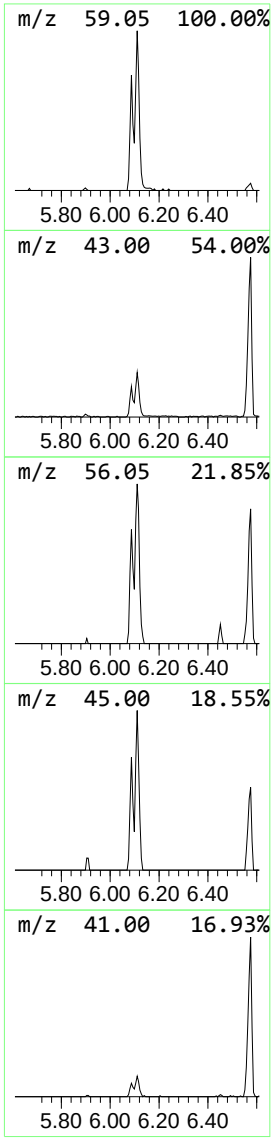
****

Peak Number 4 Oxetane, 2,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.110	3.57 ng	127173	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	74
2	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	72
3	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	50
4	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	50
5	3-Methyl-oxirane-2-carboxylic ac...	116	C5H8O3	1000194-20-4	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

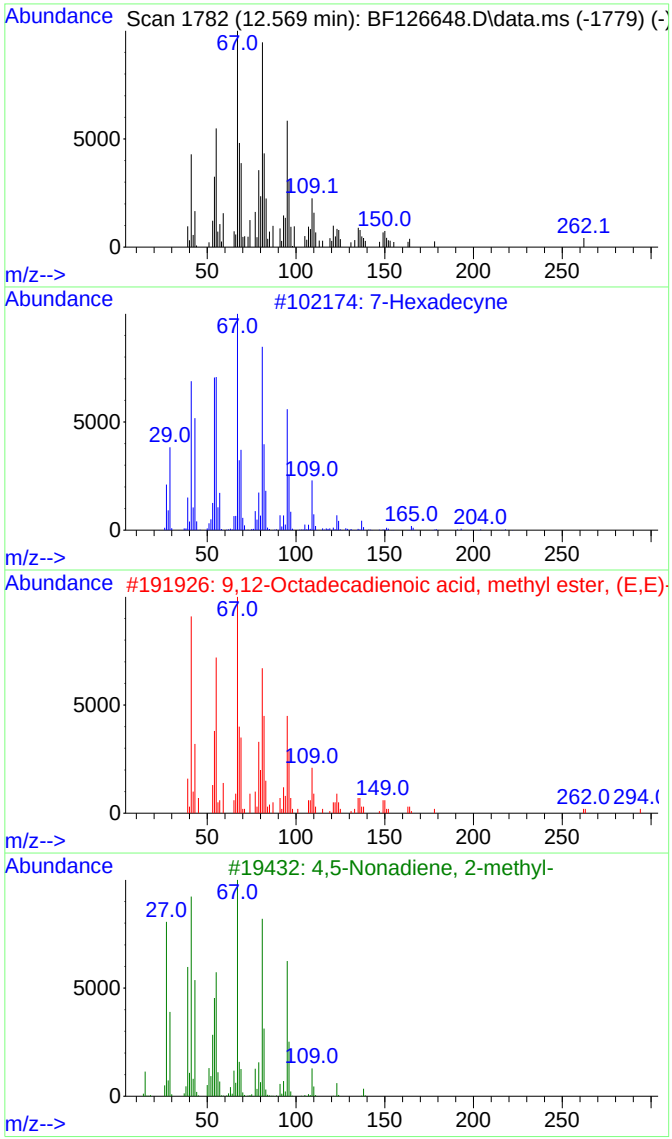
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

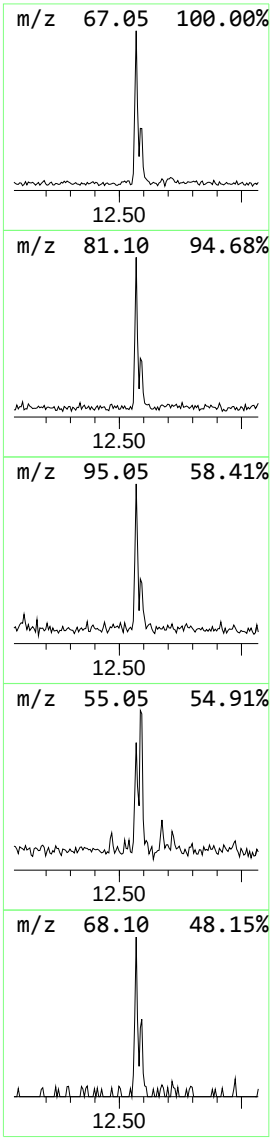
****

Peak Number 5 7-Hexadecyne Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	2.36 ng	115504	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecyne	222	C16H30	074685-28-2	80
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	76
3	4,5-Nonadiene, 2-methyl-	138	C10H18	055956-32-6	64
4	5-Undecyne	152	C11H20	002294-72-6	64
5	9,12-Octadecadien-1-ol, (Z,Z)-	266	C18H34O	000506-43-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

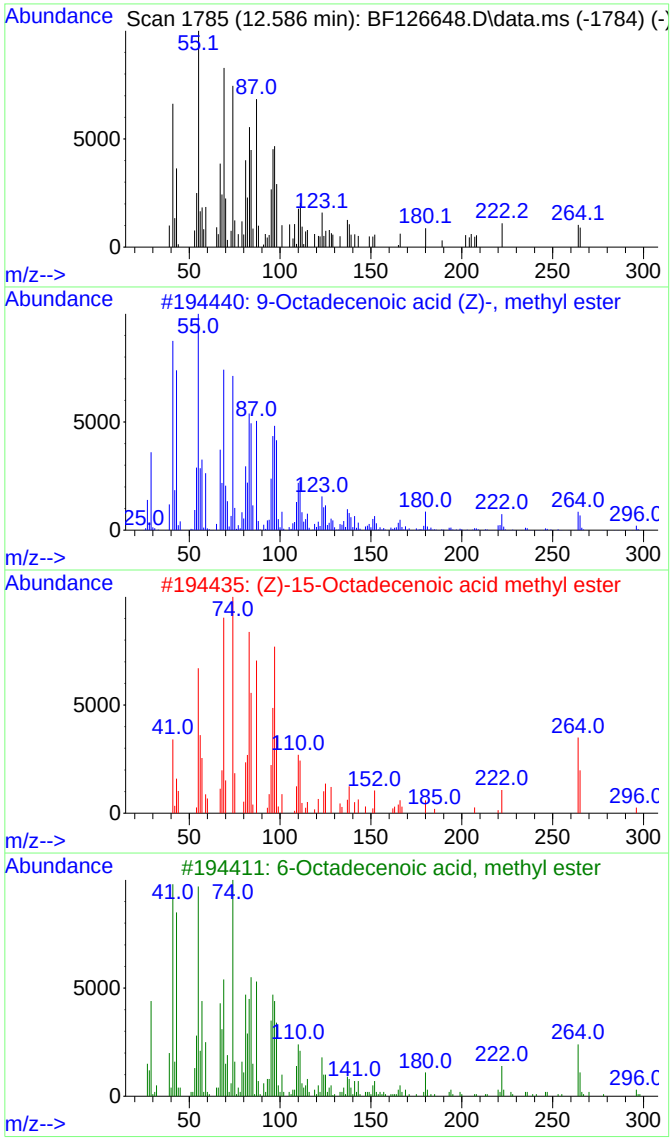
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

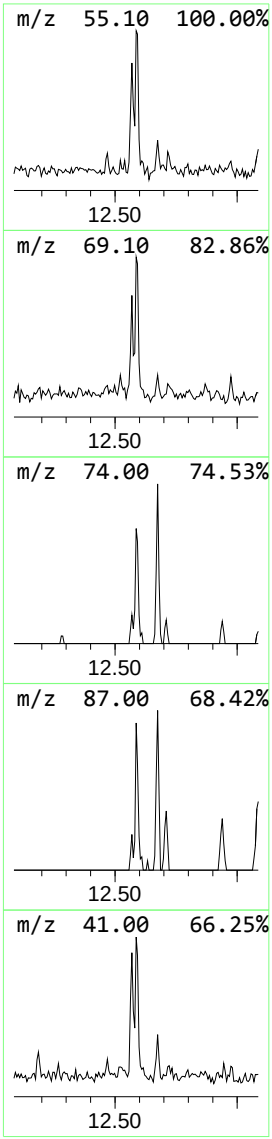
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	2.28 ng	111709	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	86
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	68
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	68
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
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Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

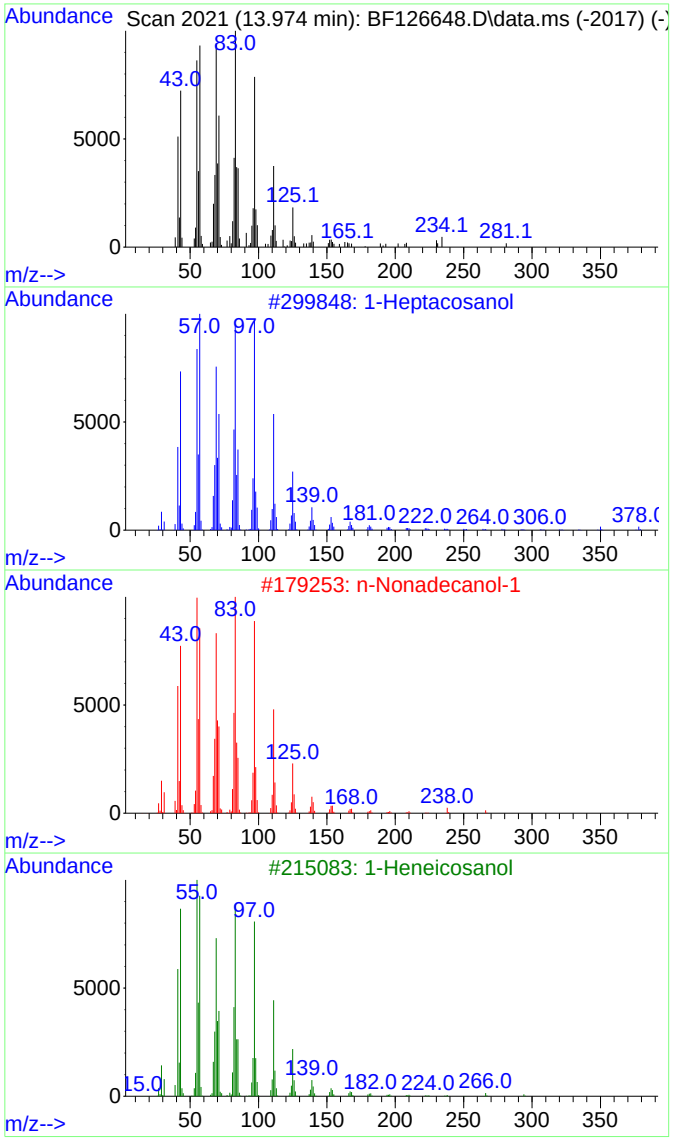
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

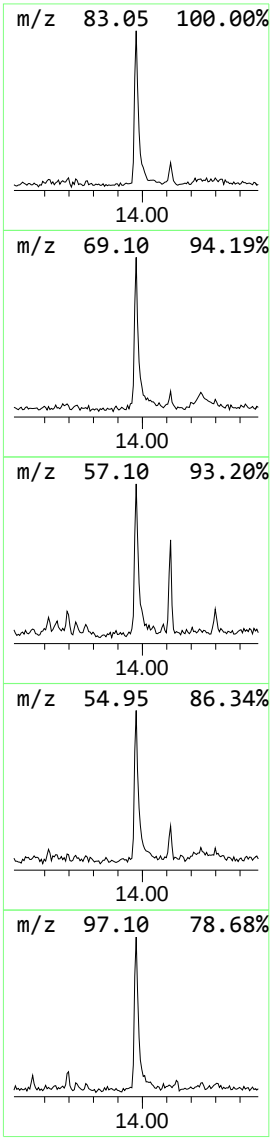
****

Peak Number 7 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	7.92 ng	284183	Chrysene-d12	14.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

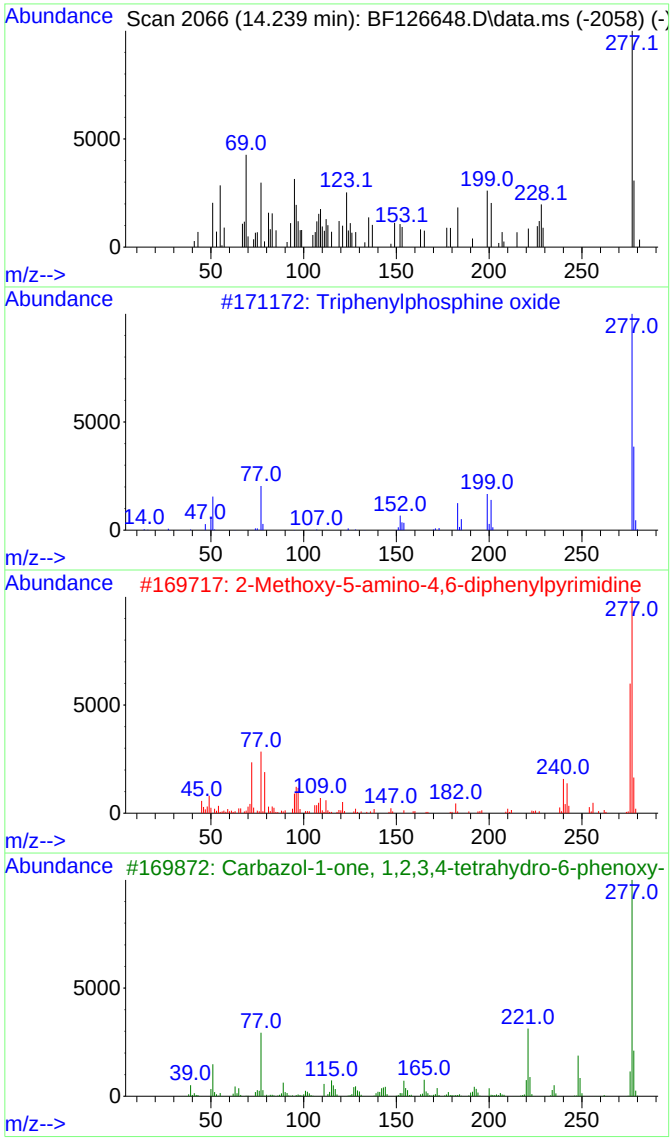
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

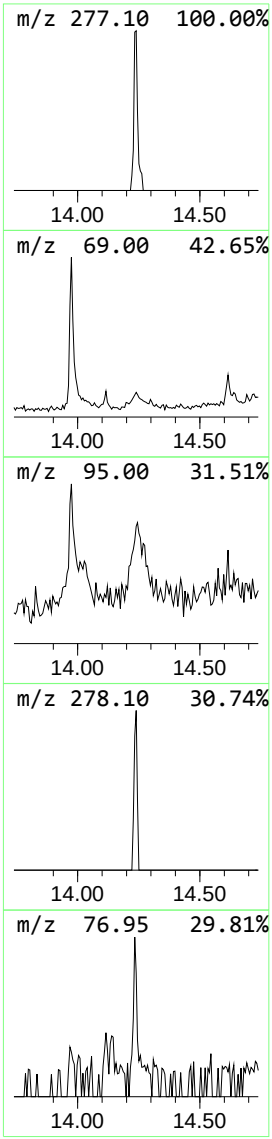
****

Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.239	2.16 ng	77609	Chrysene-d12	14.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	60
2	2-Methoxy-5-amino-4,6-diphenylpy...	277	C17H15N3O	076891-83-3	35
3	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	27
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	25
5	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	23





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Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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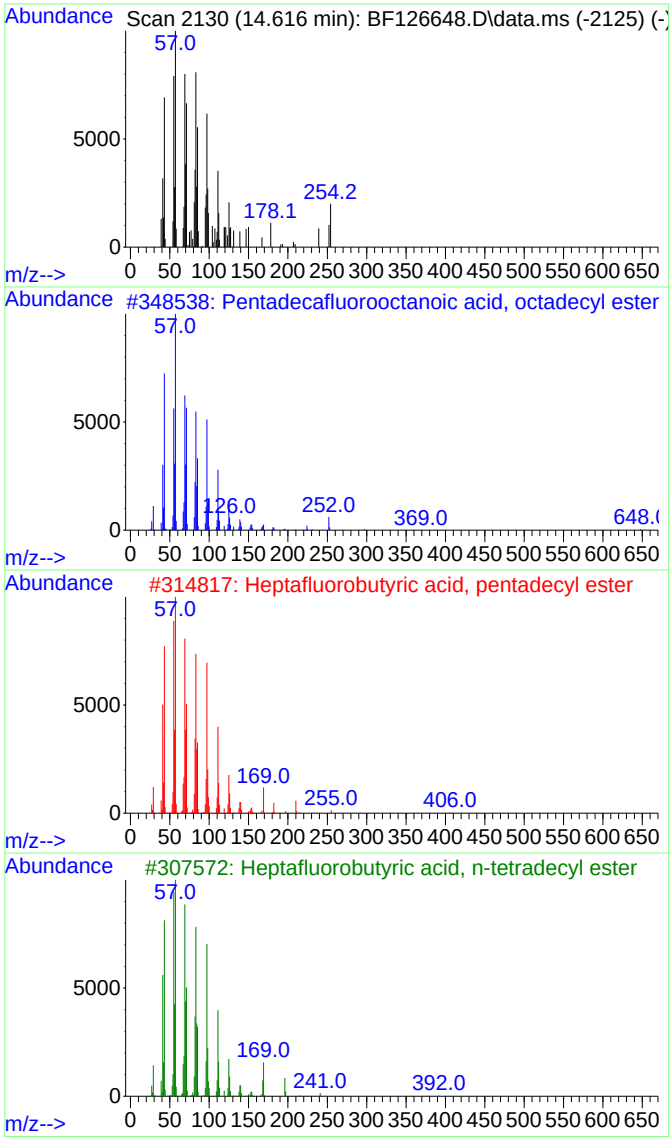
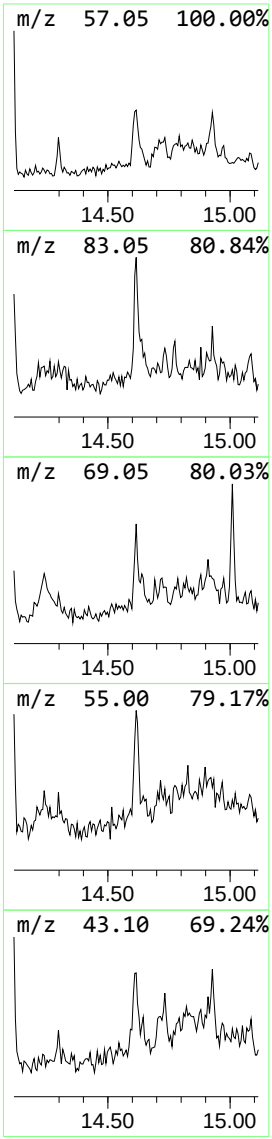
Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	2.08 ng	74657	Chrysene-d12	14.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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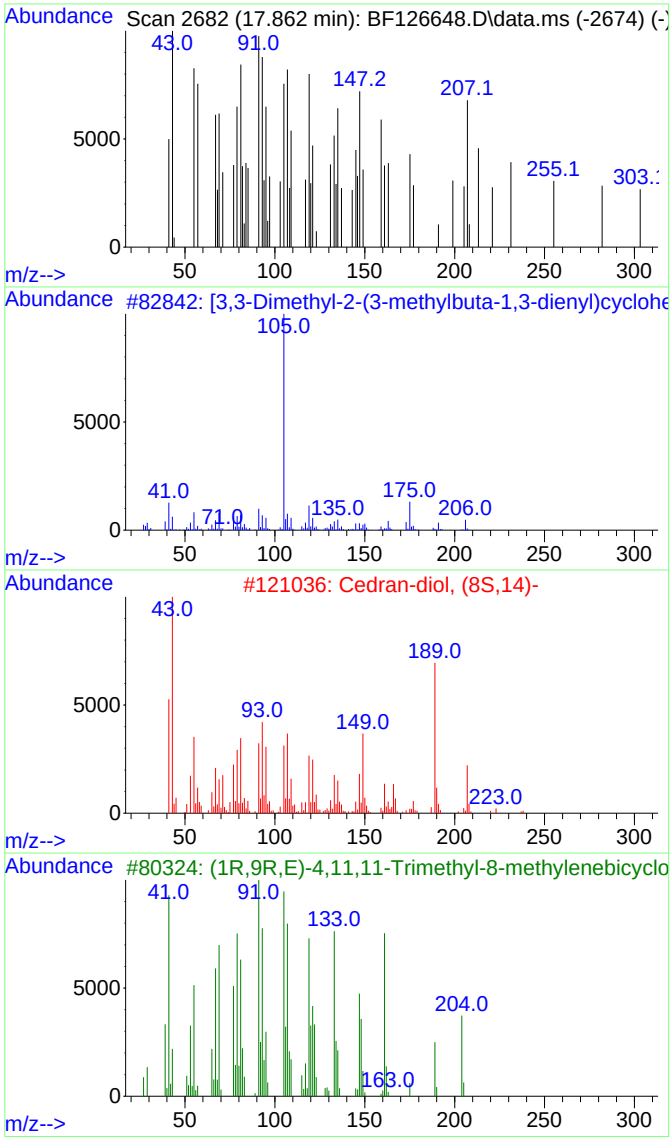
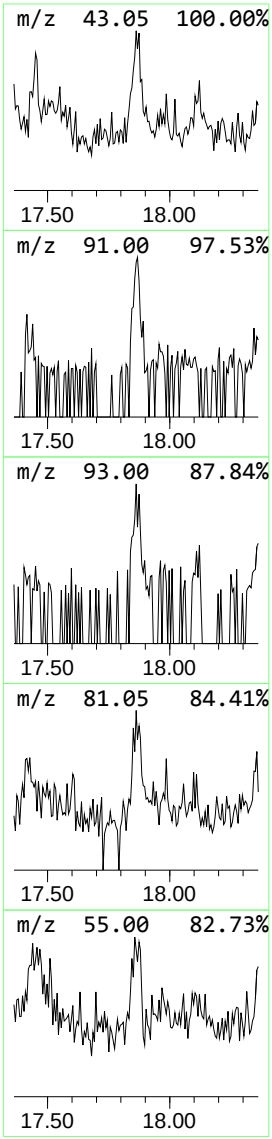
Peak Number 10 unknown17.862 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.862	2.18 ng	69926	Perylene-d12	15.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[3,3-Dimethyl-2-(3-methylbuta-1,...	206	C14H22O	1000195-13-8	35
2	Cedran-diol, (8S,14)-	238	C15H26O2	062600-05-9	35
3	(1R,9R,E)-4,11,11-Trimethyl-8-me...	204	C15H24	068832-35-9	22
4	Longifolene	204	C15H24	000475-20-7	22
5	Icosa-9,11-diyne	274	C20H34	028393-07-9	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126648.D
Acq On : 24 Jan 2022 19:24
Operator : CG/JU
Sample : N1188-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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...	2.305	53.2	ng	1897690	1	6.963	713177	20.0
2-Pentanone, 4-...	5.199	3.6	ng	128319	1	6.963	713177	20.0
Hexylene glycol	6.087	2.4	ng	83812	1	6.963	713177	20.0
Oxetane, 2,2,4-...	6.110	3.6	ng	127173	1	6.963	713177	20.0
7-Hexadecyne	12.569	2.4	ng	115504	4	11.492	980238	20.0
9-Octadecenoic ...	12.586	2.3	ng	111709	4	11.492	980238	20.0
1-Heptacosanol	13.974	7.9	ng	284183	5	14.139	717829	20.0
Triphenylphosph...	14.239	2.2	ng	77609	5	14.139	717829	20.0
Pentadecafluoro...	14.616	2.1	ng	74657	5	14.139	717829	20.0
unknown17.862	17.862	2.2	ng	69926	6	15.663	641014	20.0