LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	9	20	28	rVB	1370312	1914446	27.66%	3.404%
2	2.310	32	38	44	rBV2	74675	107514	1.55%	0.191%
3	4.469	395	405	409	rBV	2928490	3530990	51.01%	6.279%
4	5.093	503	511	514	rBV	3405974	4892144	70.68%	8.699%
5	5.481	572	577	580	rBV	4266712	3872600	55.95%	6.886%
6	6.487	742	748	751	rBV	5287970	5497737	79.43%	9.776%
7	6.851	807	810	814	rBV	1378949	1126247	16.27%	2.003%
8	7.416	900	906	909	rBV	3928257	3887916	56.17%	6.913%
9	8.039	1007	1012	1022	rBV	495760	592516	8.56%	1.054%
10	8.133	1023	1028	1032	rBV	1569123	1345202	19.43%	2.392%
11	9.210	1205	1211	1214	rBV	7165075	6921815	100.00%	12.308%
12	9.886	1319	1326	1330	rBV	1533112	1388037	20.05%	2.468%
13	10.322	1397	1400	1402	rVB	121009	90259	1.30%	0.160%
14	10.545	1432	1438	1440	rBV	84230	119864	1.73%	0.213%
15	10.675	1455	1460	1465	rBV	1338265	1271814	18.37%	2.261%
16	10.763	1472	1475	1478	rBV	73621	86843	1.25%	0.154%
17	10.792	1478	1480	1482	rBV	162831	171899	2.48%	0.306%
18	10.945	1499	1506	1509	rBV	144459	233492	3.37%	0.415%
19	10.986	1510	1513	1517	rBV2	168136	243449	3.52%	0.433%
20	11.239	1553	1556	1558	rBV2	217031	192971	2.79%	0.343%
21	11.269	1558	1561	1564	rVV	259879	325435	4.70%	0.579%
22	11.374	1575	1579	1581	rBV	1309264	1169528	16.90%	2.080%
23	11.422	1584	1587	1592	rVV2	220997	401500	5.80%	0.714%
24	11.522	1601	1604	1607	rBV3	134516	184730	2.67%	0.328%
25	11.557	1607	1610	1613	rBV	234910	292428	4.22%	0.520%
26	11.680	1627	1631	1635	rBV	295026	551348	7.97%	0.980%
27	11.833	1654	1657	1662	rBV2	300165	476225	6.88%	0.847%
28	11.904	1666	1669	1672	rBV2	222181	219277	3.17%	0.390%
29	11.933	1672	1674	1677	rBV2	143251	133341	1.93%	0.237%
30	11.969	1677	1680	1685	rBV	302337	551371	7.97%	0.980%
31	12.080	1696	1699	1702	rBV	366423	443570	6.41%	0.789%
32	12.192	1716	1718	1721	rBV2	141701	150591	2.18%	0.268%
33	12.233	1722	1725	1727	rBV2	245627	321210	4.64%	0.571%
34	12.357	1743	1746	1750	rBV2	466336	539982	7.80%	0.960%
35	12.398	1751	1753	1756	rVB2	331612	283148	4.09%	0.503%
36	12.469	1762	1765	1768	rBV	431979	492491	7.12%	0.876%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.580	1782	1784	1787	rBV2	265636	293877	4.25%	0.523%
38	12.610	1787	1789	1794	rVV	297335	491004	7.09%	0.873%
39	12.657	1795	1797	1799	rVB	286294	221276	3.20%	0.393%
40	12.816	1821	1824	1826	rBV	299100	299636	4.33%	0.533%
41	12.839	1826	1828	1831	rVV	326786	356050	5.14%	0.633%
42	12.874	1831	1834	1840	rVB	398002	594791	8.59%	1.058%
43	12.963	1845	1849	1852	rBV	7047743	6230619	90.01%	11.079%
44	13.221	1891	1893	1899	rVB3	410234	583316	8.43%	1.037%
45	13.868	2000	2003	2013	rVB4	424092	821256	11.86%	1.460%
46	14.015	2024	2028	2030	rVB	1147791	1035970	14.97%	1.842%
47	14.662	2135	2138	2141	rVB	246466	192972	2.79%	0.343%
48	15.480	2273	2277	2281	rBV	672945	750758	10.85%	1.335%
49	15.957	2355	2358	2365	rBV2	214018	343282	4.96%	0.610%

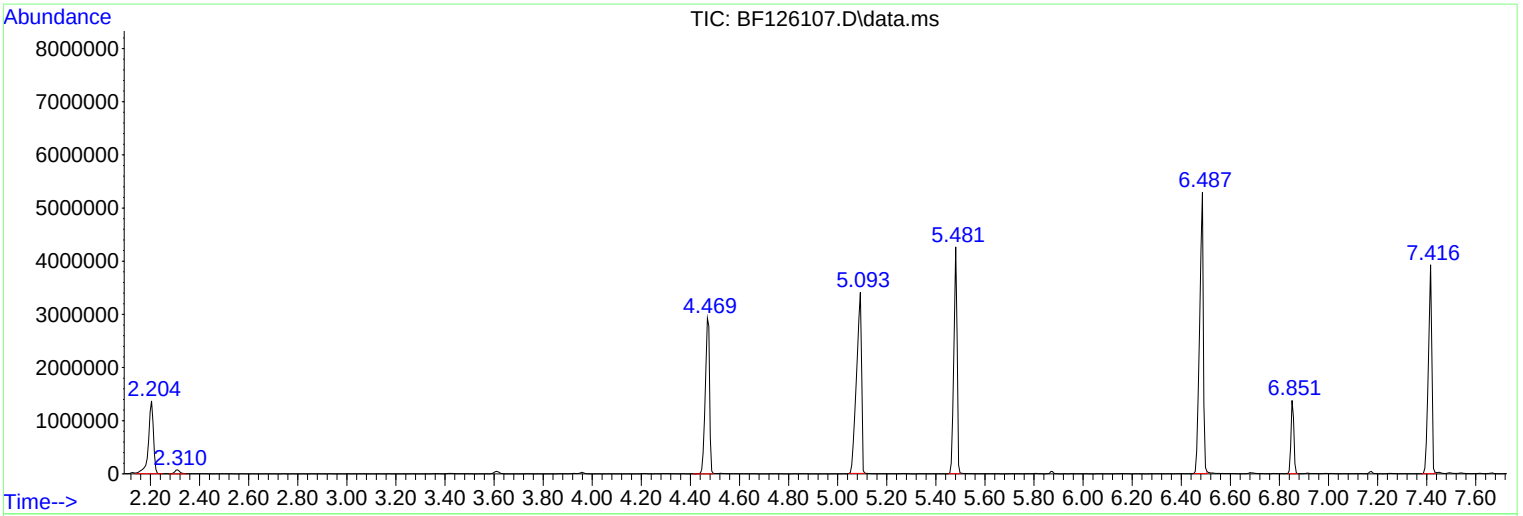
Sum of corrected areas: 56238737

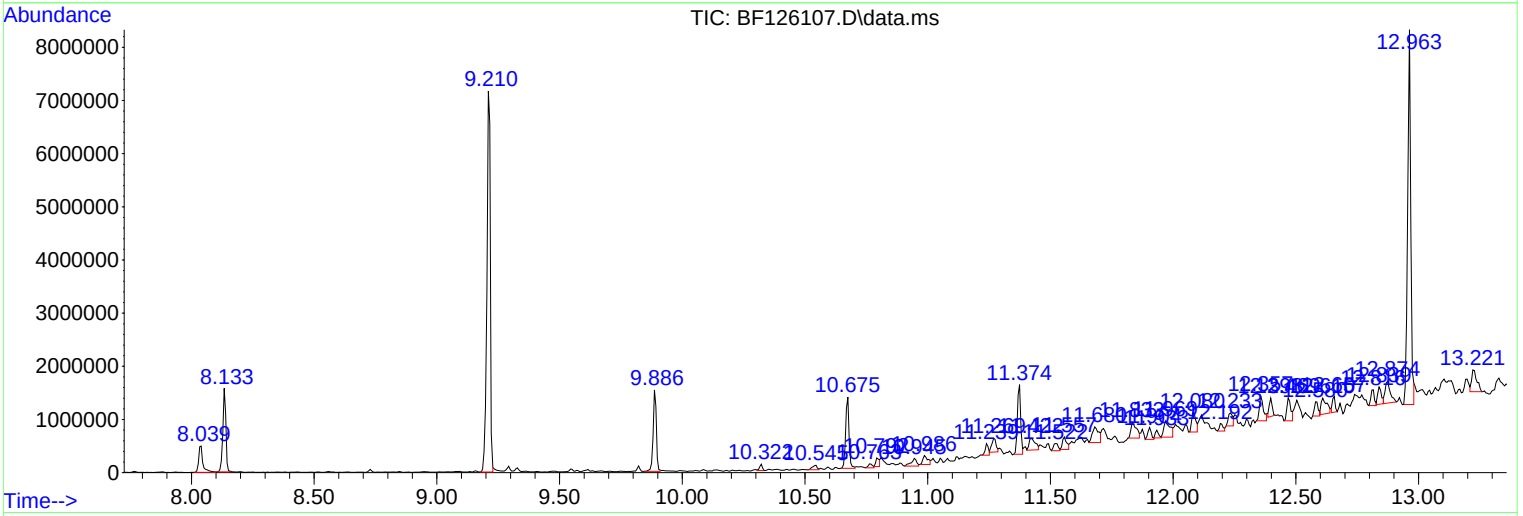
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

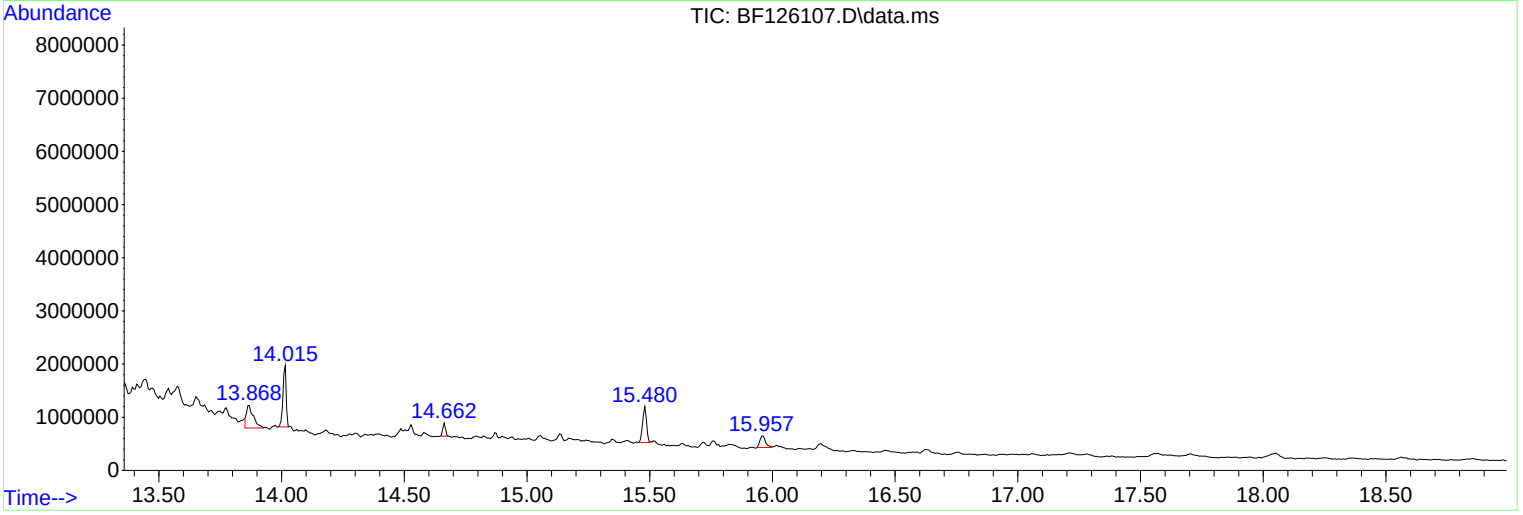
Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

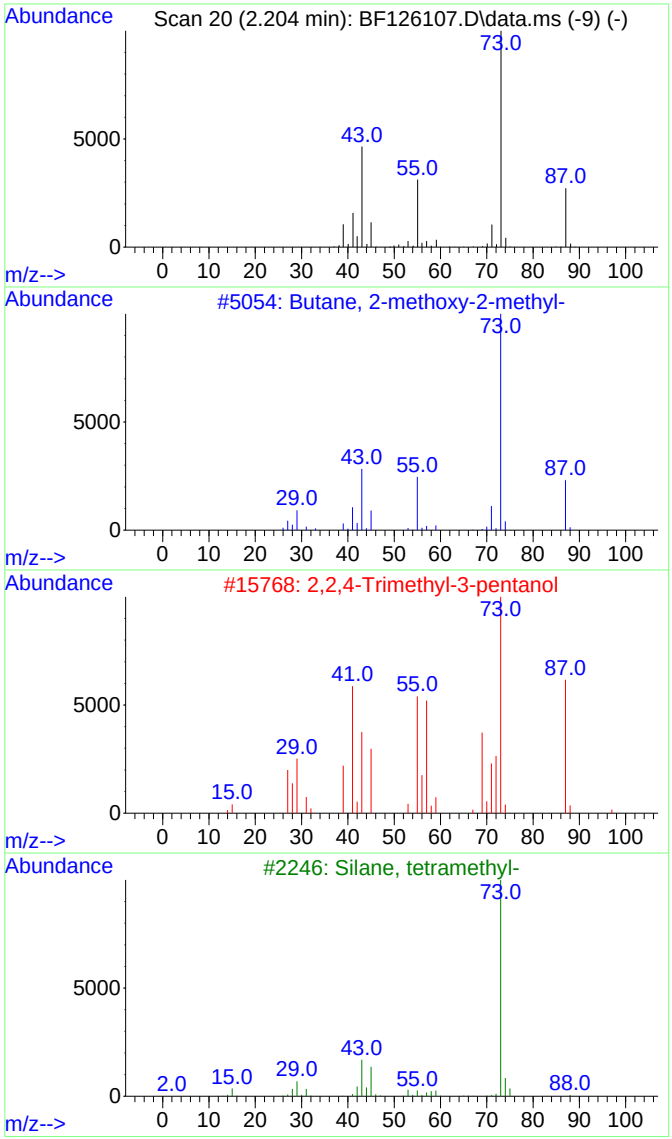
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

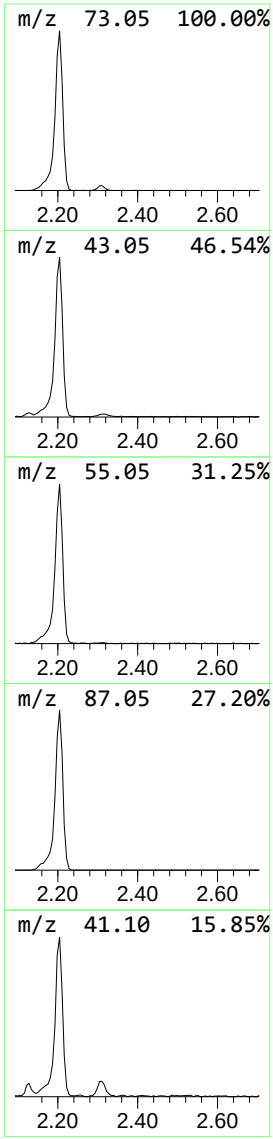
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	34.00 ng	1914450	1,4-Dichlorobenzene-d4	6.851

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

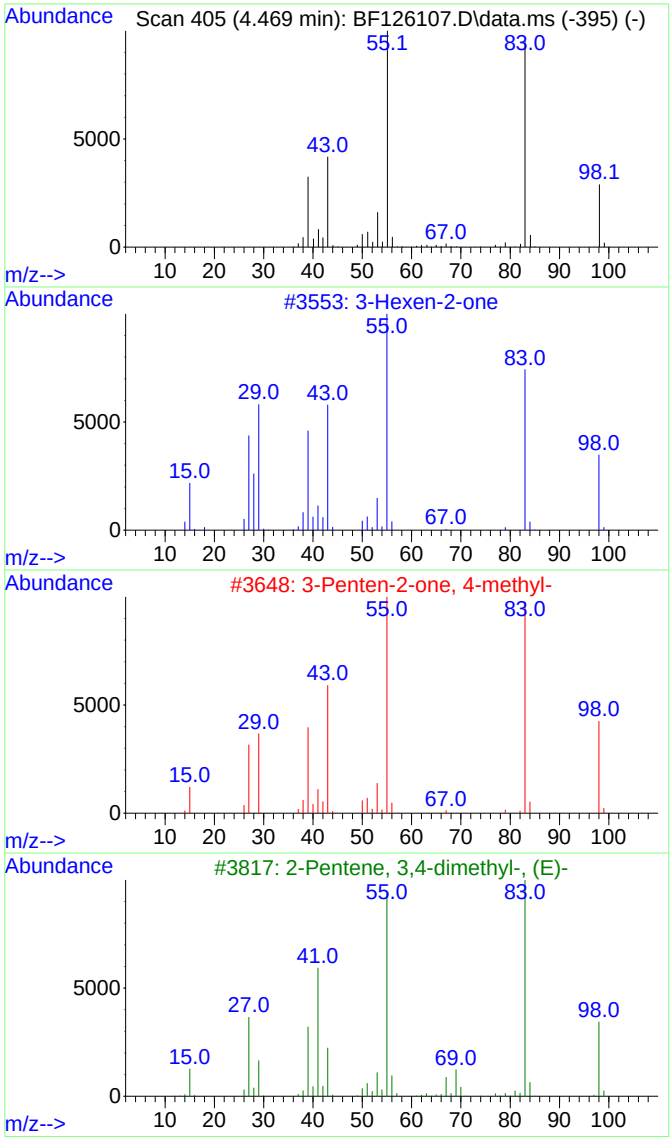
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

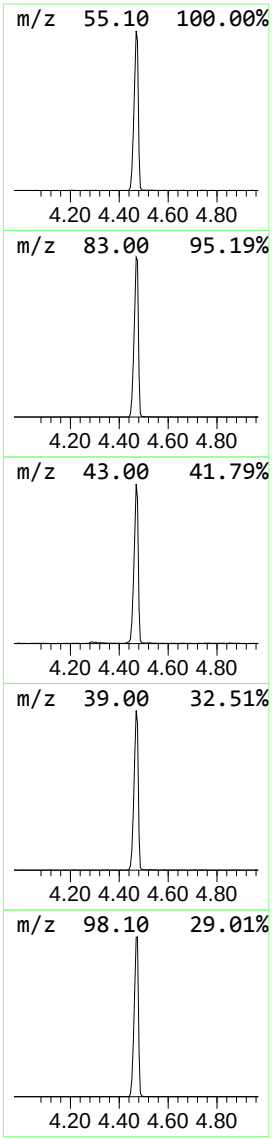
****

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	62.70 ng	3530990	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

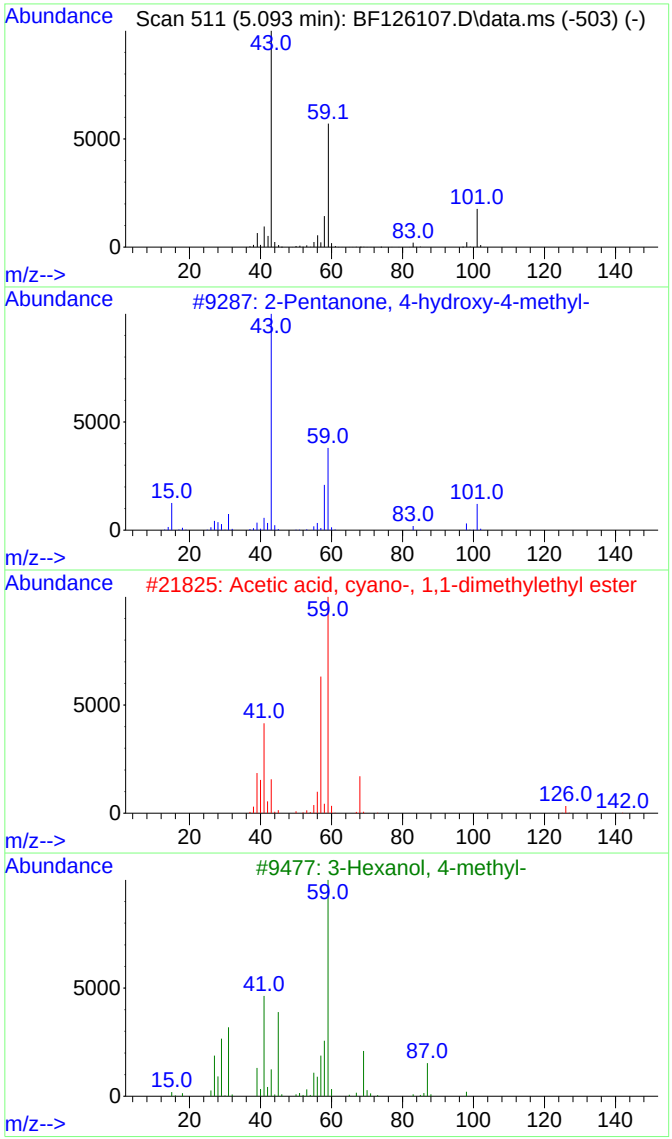
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

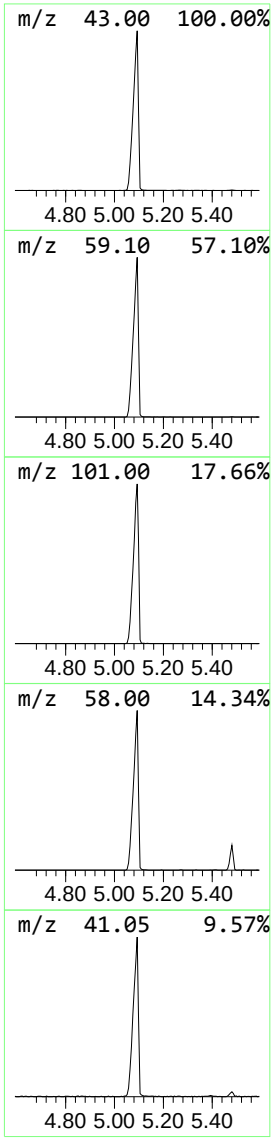
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	86.88 ng	4892140	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

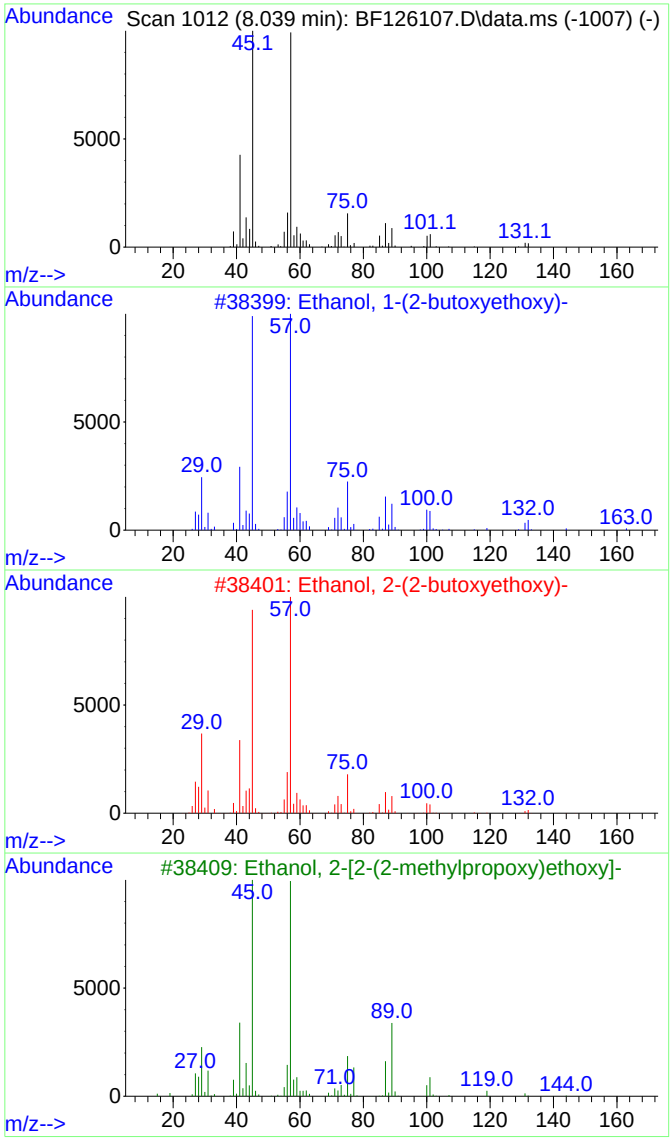
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

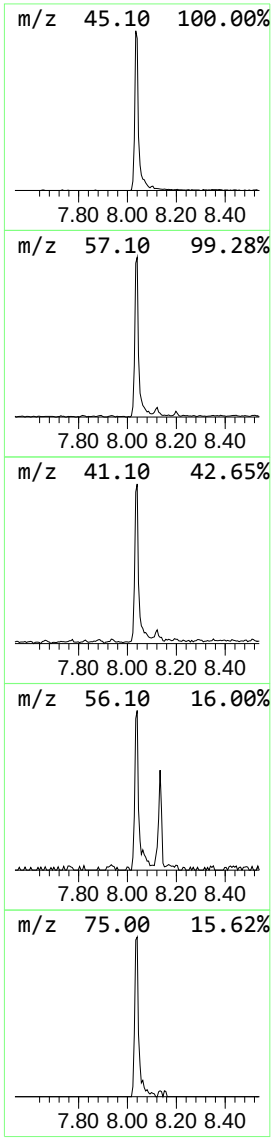
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	8.81 ng	592516	Naphthalene-d8	8.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

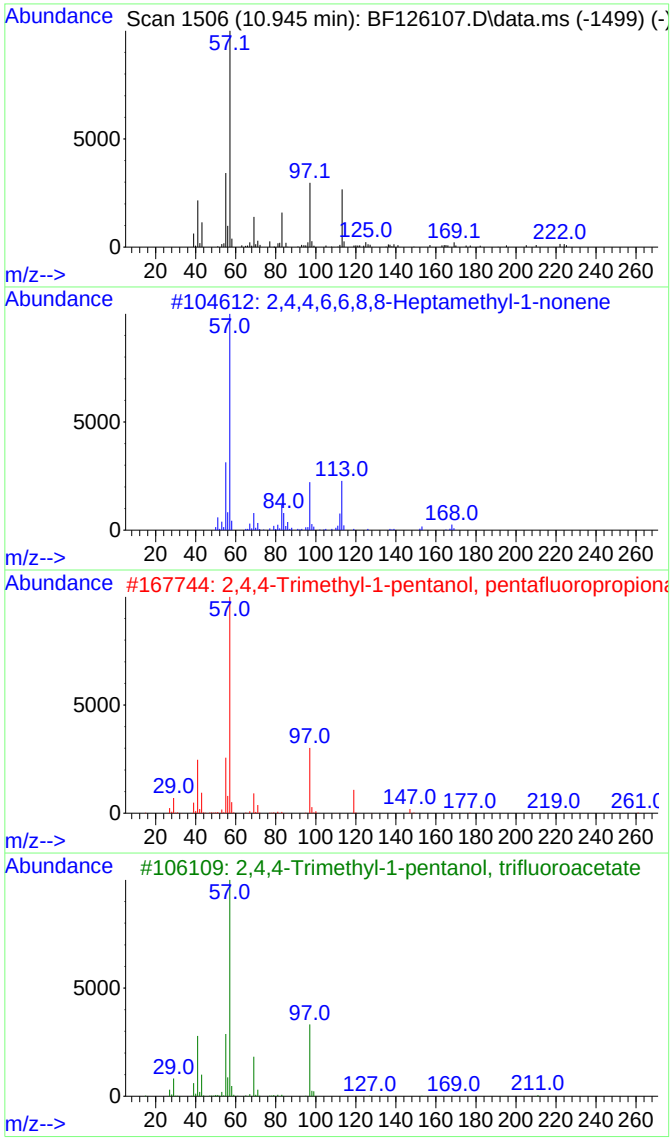
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

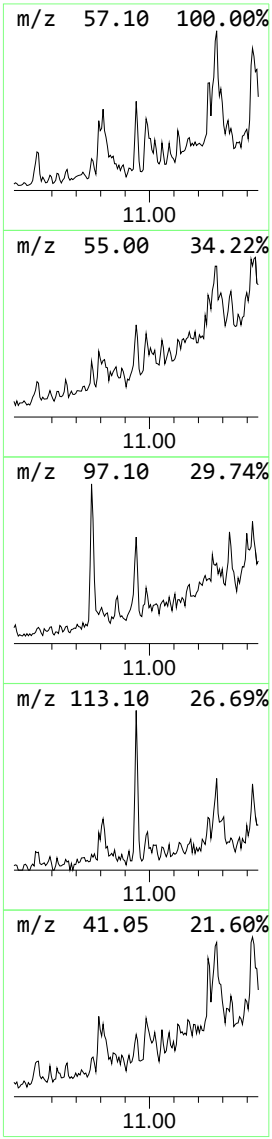
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	3.99 ng	233492	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	47
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	47
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	40
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1010365-01-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

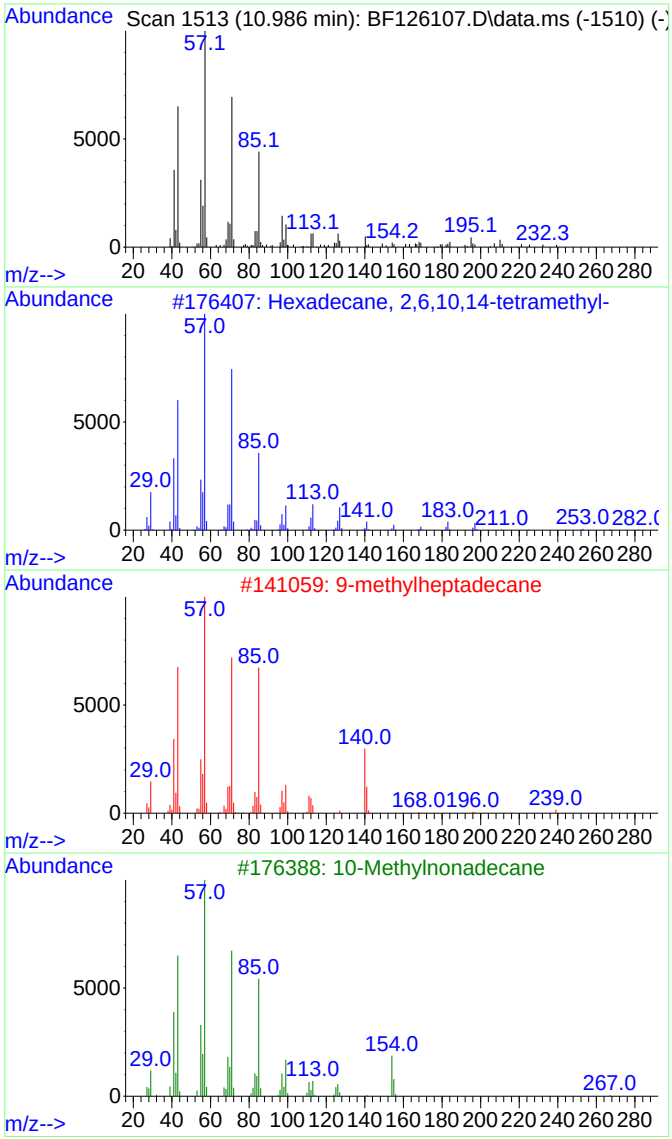
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

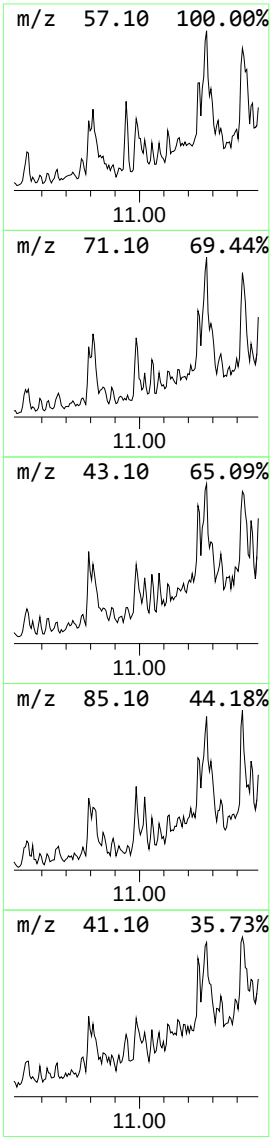
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.986	4.16 ng	243449	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
2	9-methylheptadecane	254	C18H38	026741-18-4	80
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5	Tridecane	184	C13H28	000629-50-5	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

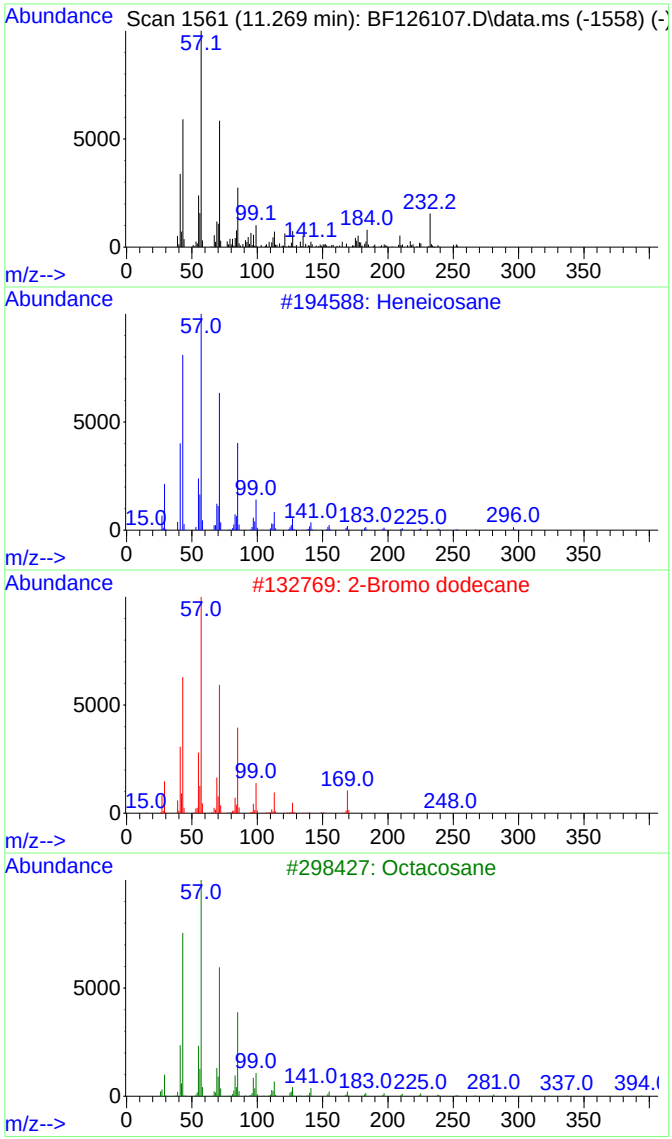
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

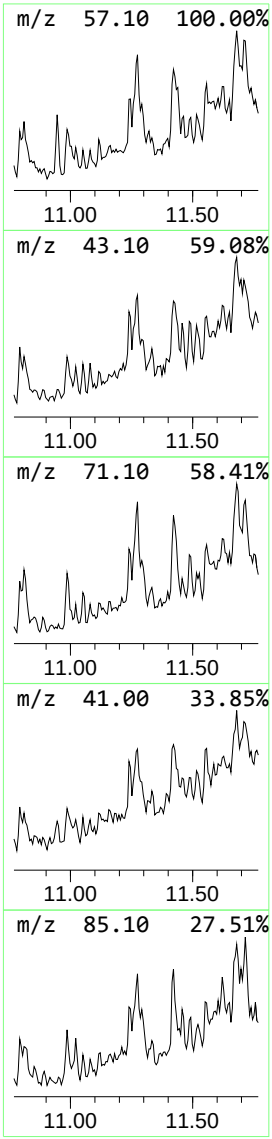
****

Peak Number 7 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	5.57 ng	325435	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	68
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	64
3	Octacosane	394	C28H58	000630-02-4	64
4	Eicosane	282	C20H42	000112-95-8	64
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

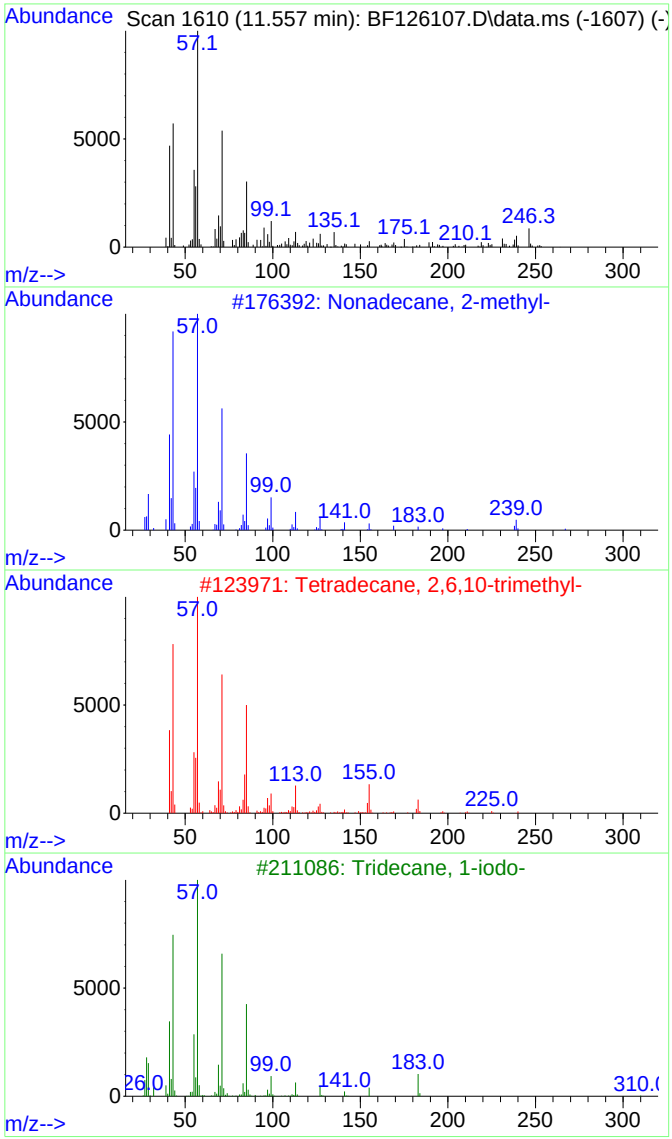
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

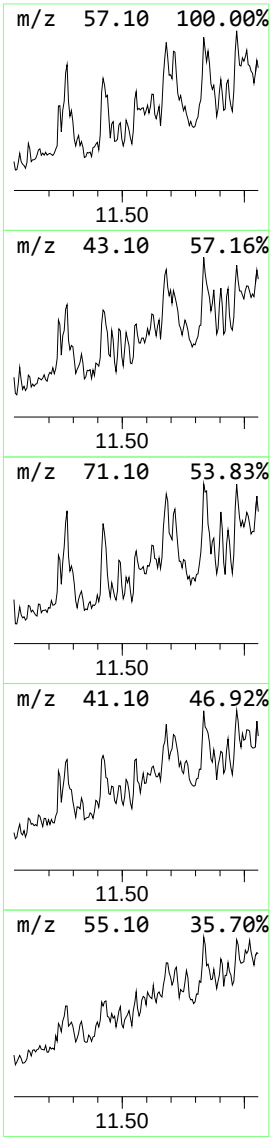
****

Peak Number 8 Nonadecane, 2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.557	5.00 ng	292428	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	74
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	68
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	62
4	Octacosane	394	C28H58	000630-02-4	62
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

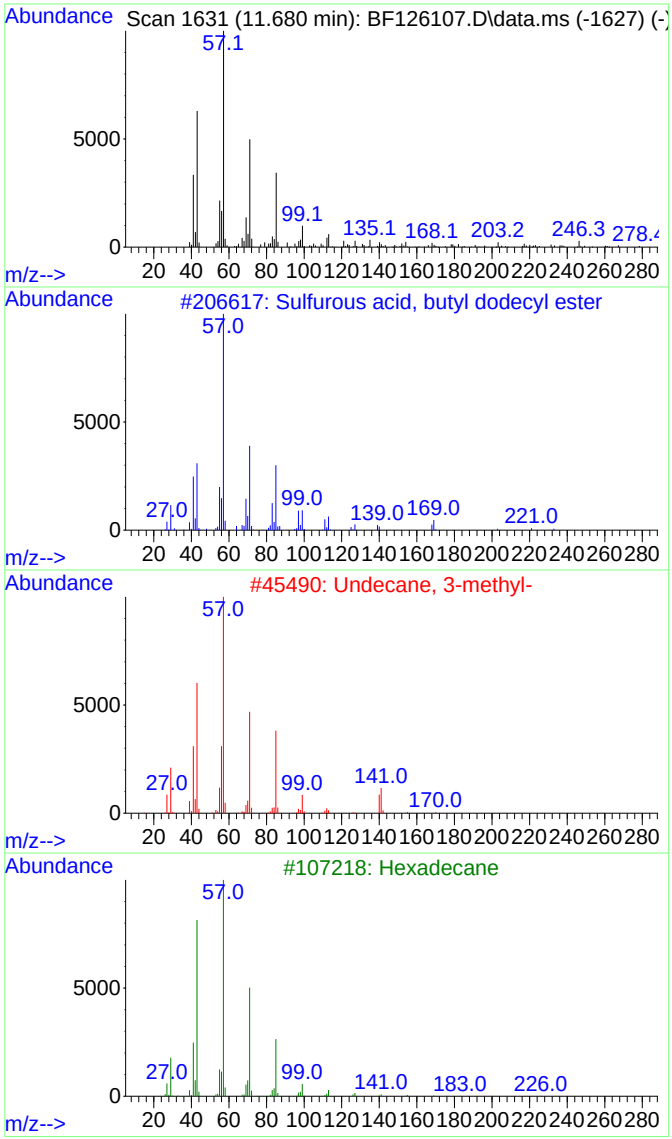
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

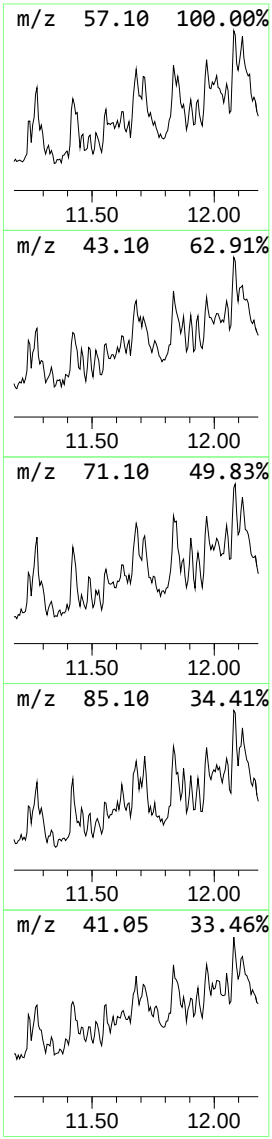
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, butyl dodec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.680	9.43 ng	551348	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2	Undecane, 3-methyl-	170	C12H26	001002-43-3	80
3	Hexadecane	226	C16H34	000544-76-3	78
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

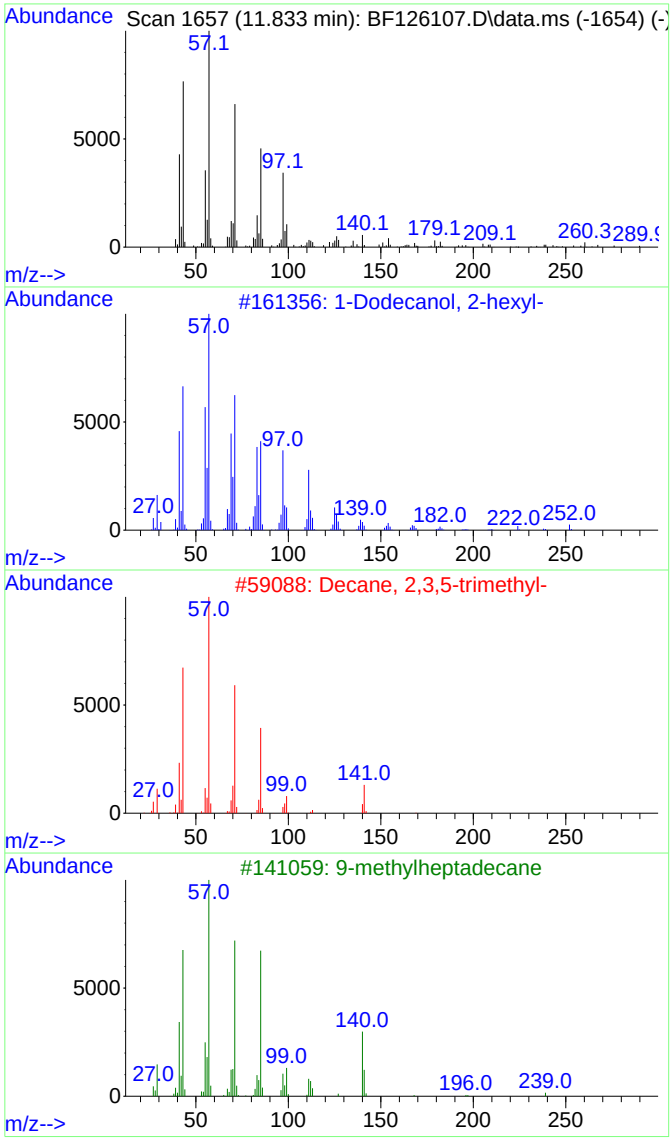
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

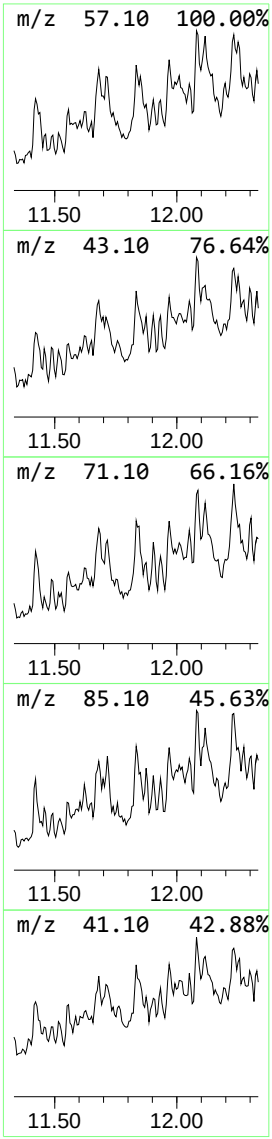
****

Peak Number 10 1-Dodecanol, 2-hexyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	8.14 ng	476225	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	78
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
3	9-methylheptadecane	254	C18H38	026741-18-4	72
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	70
5	Pentadecane	212	C15H32	000629-62-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

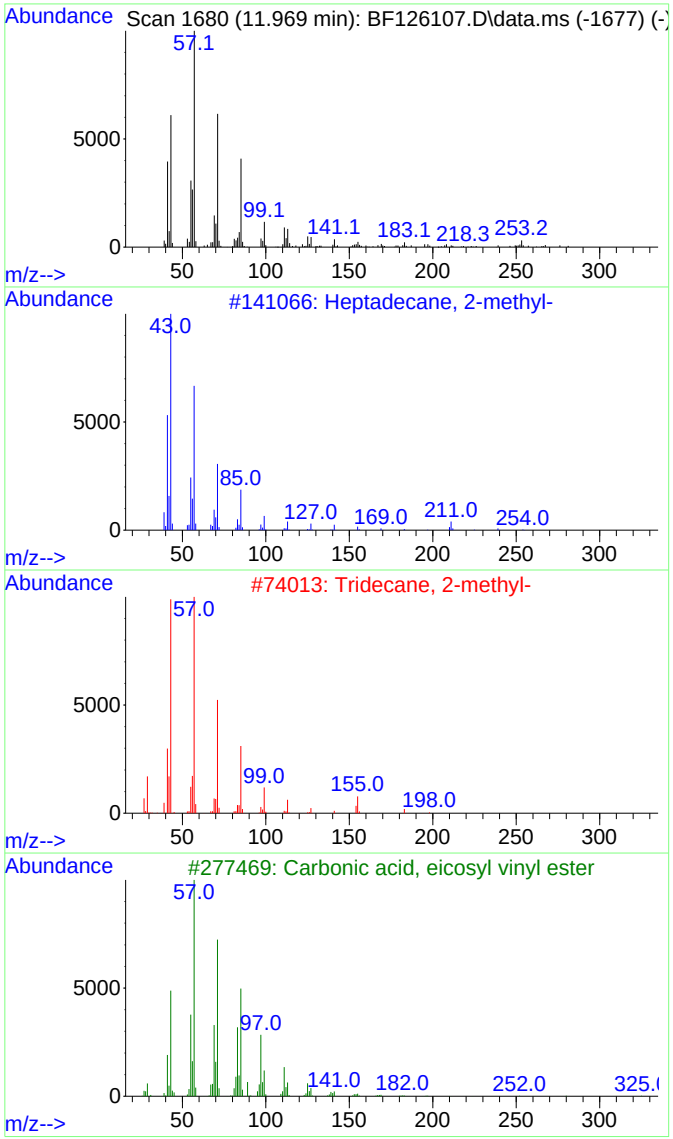
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

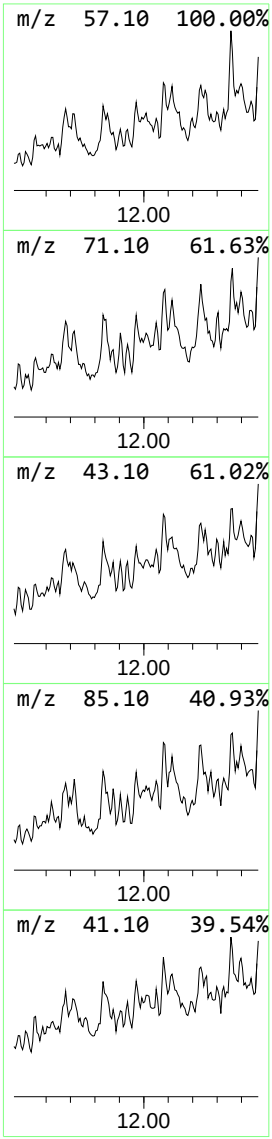
****

Peak Number 11 Heptadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	9.43 ng	551371	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	94
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	81
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
4	Heneicosane	296	C21H44	000629-94-7	74
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

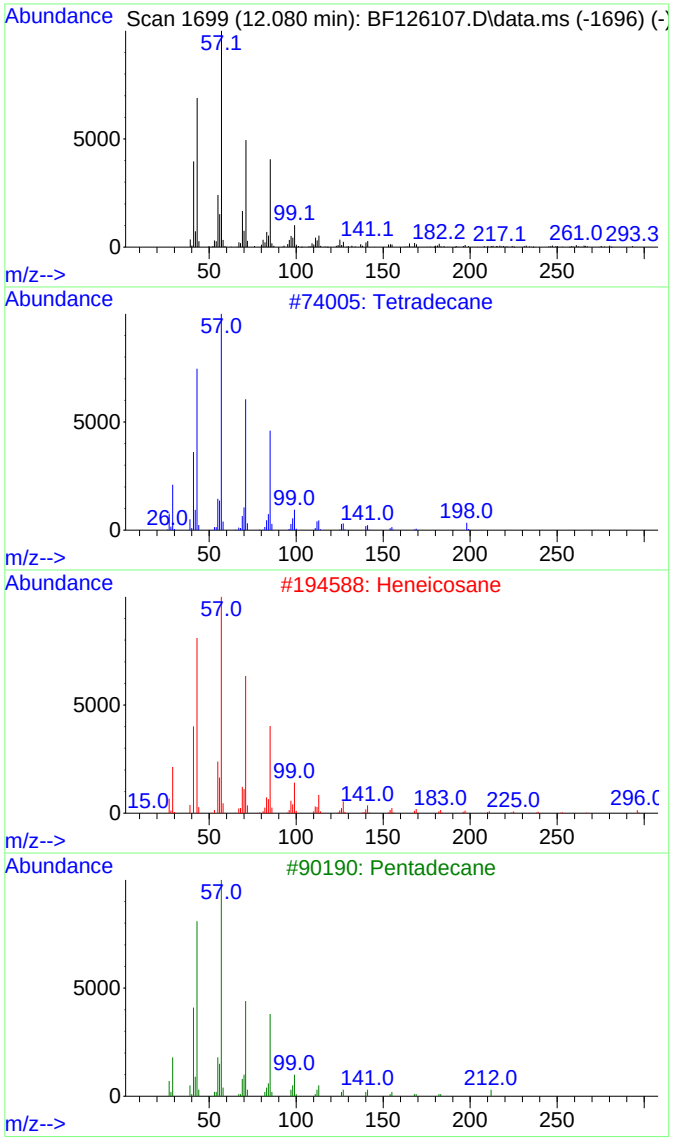
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

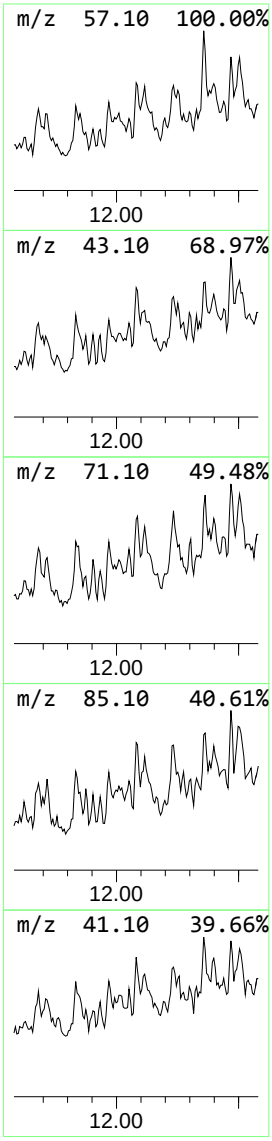
****

Peak Number 12 Tetradecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.080	7.59 ng	443570	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

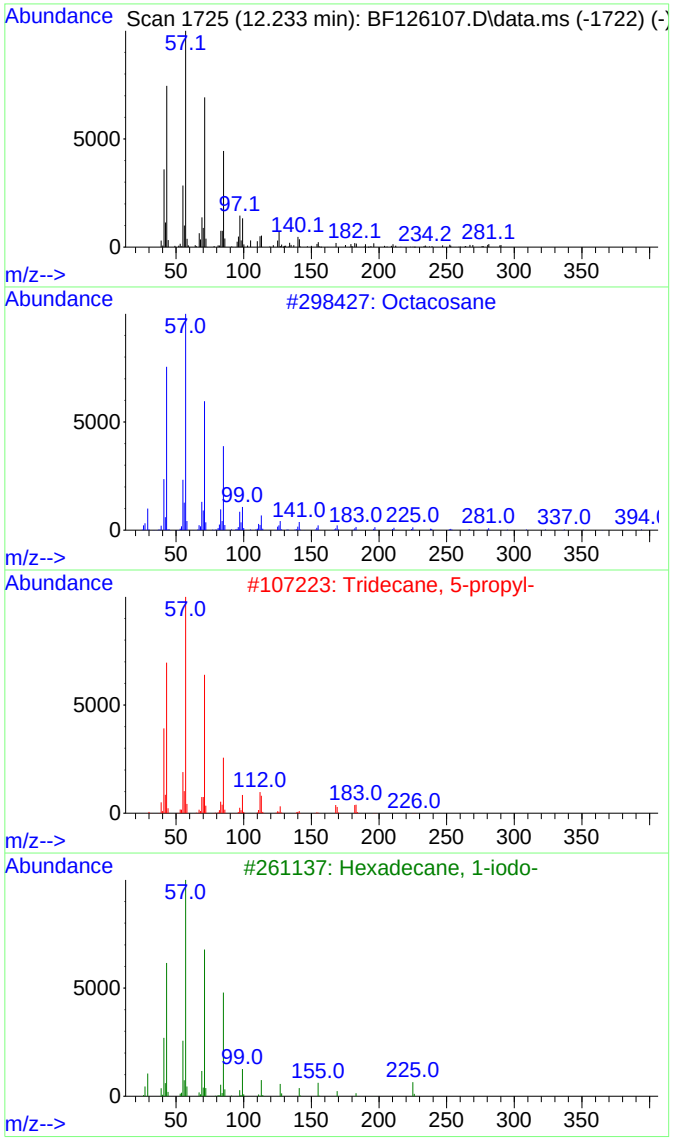
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

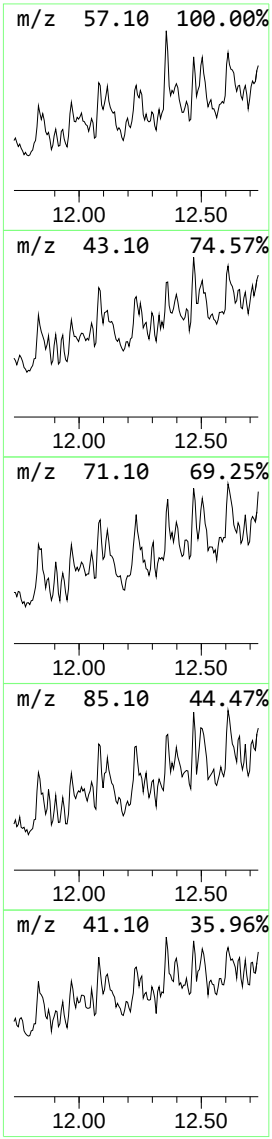
****

Peak Number 13 Octacosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	5.49 ng	321210	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

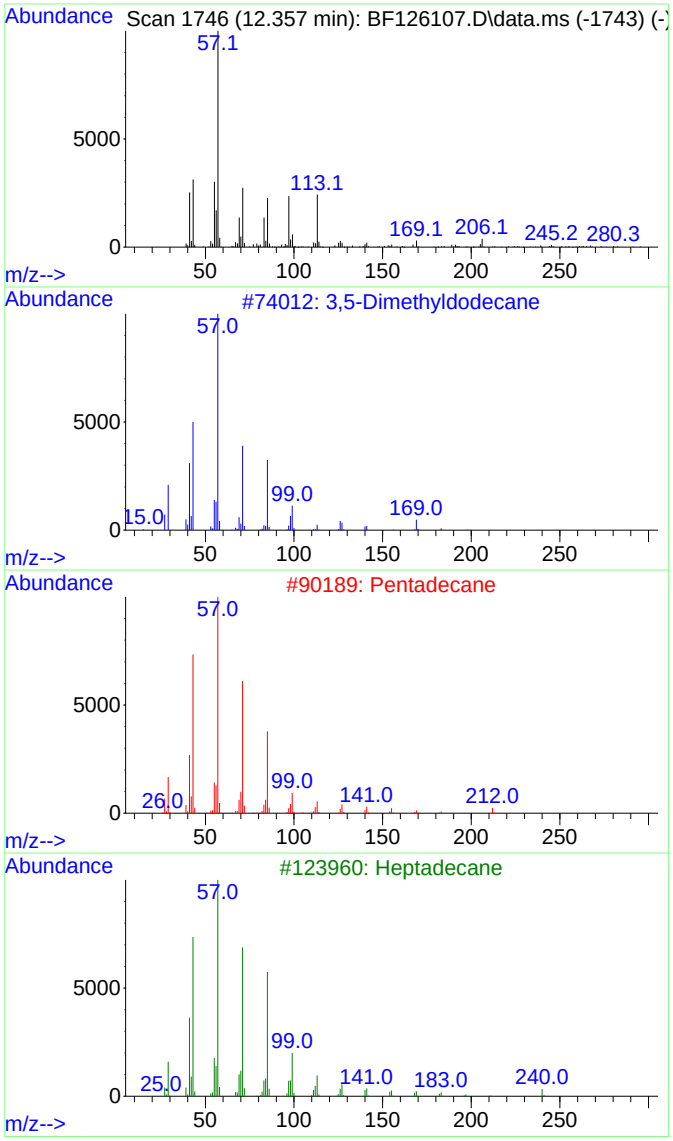
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

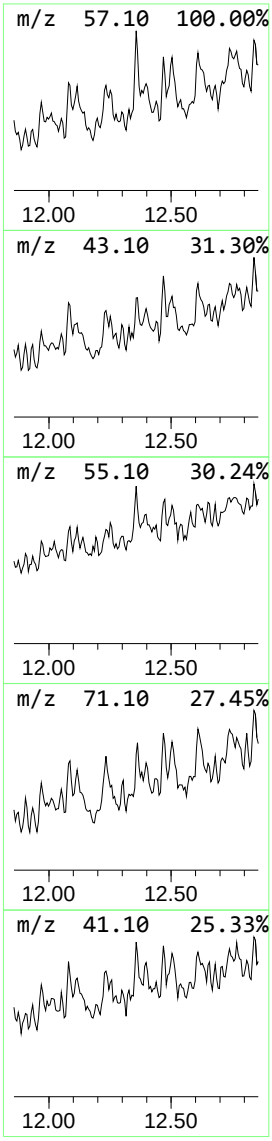
****

Peak Number 14 3,5-Dimethyldodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	9.23 ng	539982	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyldodecane	198	C14H30	107770-99-0	53
2	Pentadecane	212	C15H32	000629-62-9	38
3	Heptadecane	240	C17H36	000629-78-7	38
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38
5	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

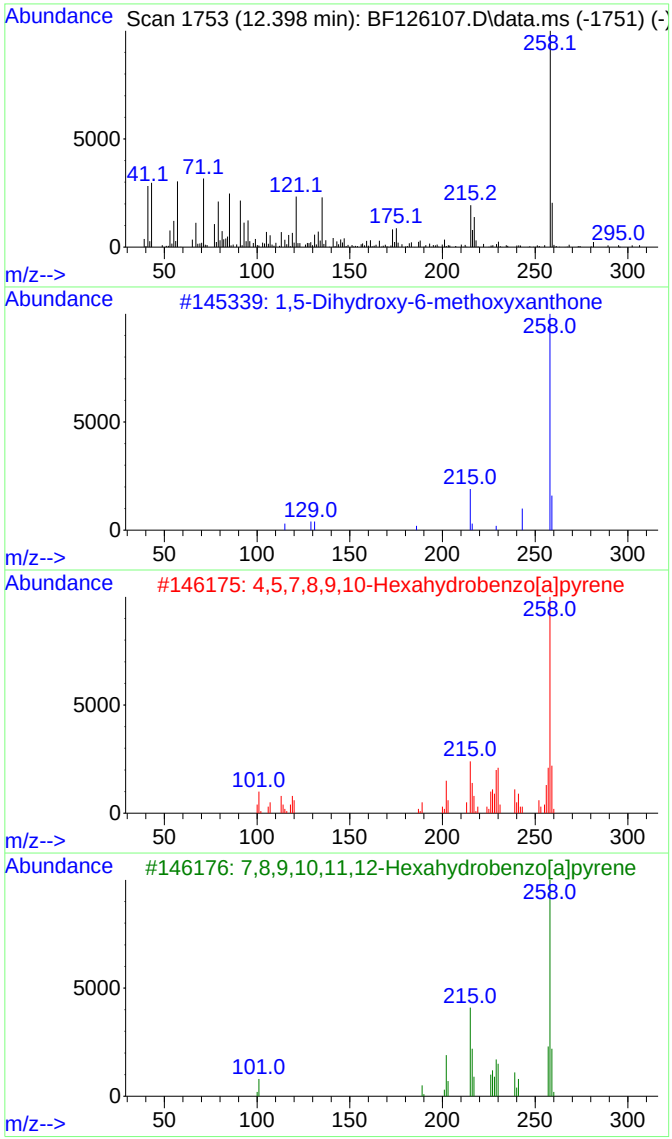
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

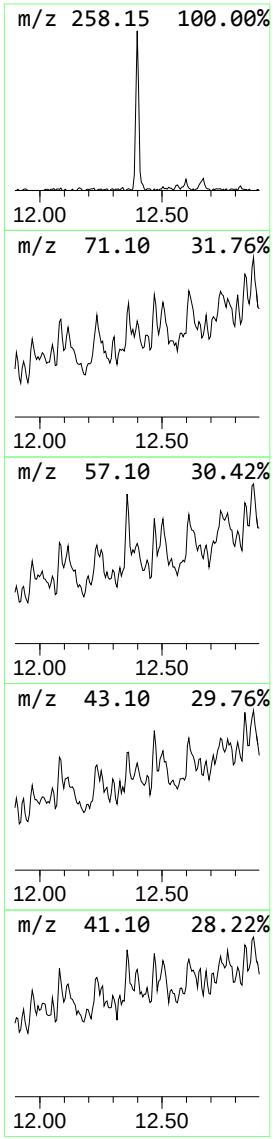
****

Peak Number 15 1,5-Dihydroxy-6-methoxyxant... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	4.84 ng	283148	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Dihydroxy-6-methoxyxanthone	258	C14H10O5	181307-35-7	64
2	4,5,7,8,9,10-Hexahydrobenzo[a]py...	258	C20H18	073712-75-1	50
3	7,8,9,10,11,12-Hexahydrobenzo[a]...	258	C20H18	073712-71-7	38
4	Benzo[1,2-b:5,4-b']bisbenzofuran	258	C18H10O2	000241-36-1	35
5	Benzo[1,2-b:3,4-b']bisbenzofuran	258	C18H10O2	000198-88-9	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

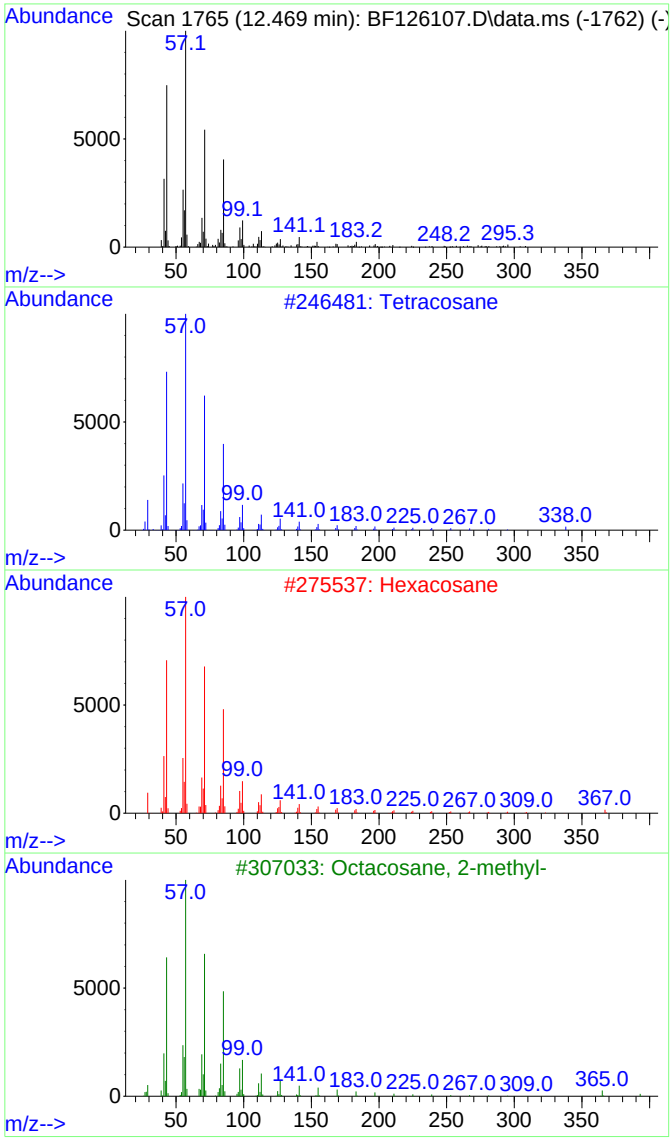
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

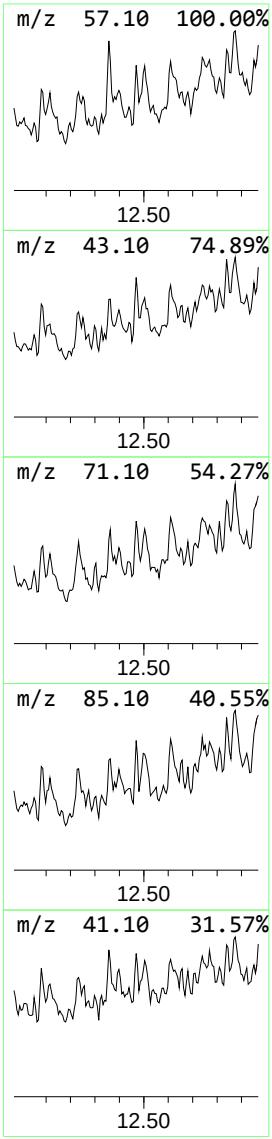
****

Peak Number 16 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	8.42 ng	492491	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

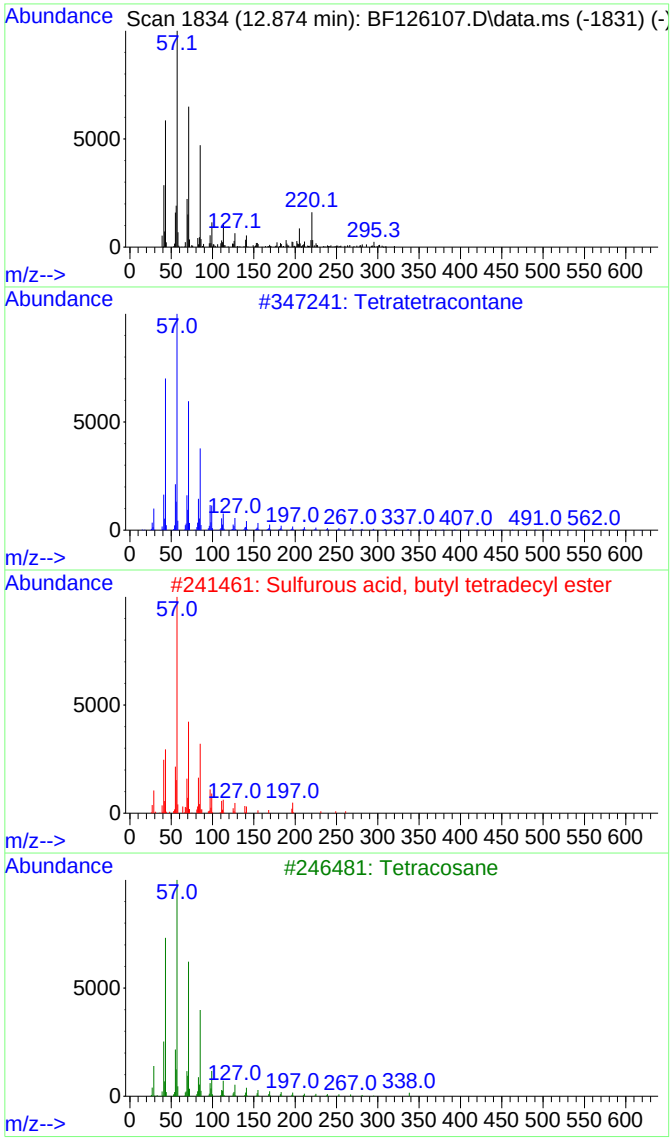
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

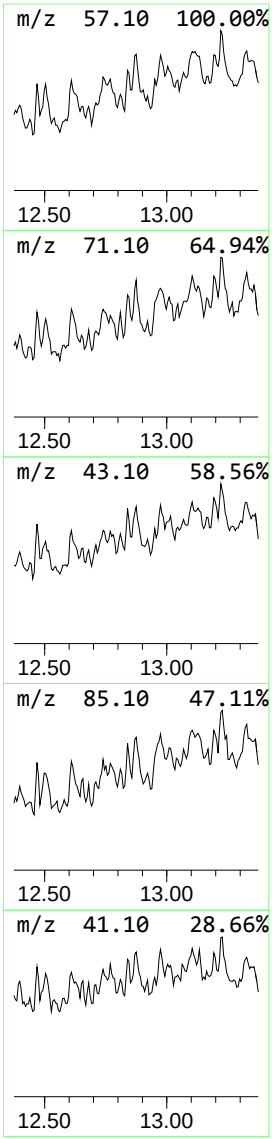
****

Peak Number 17 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	11.48 ng	594791	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	80
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	80
3	Tetracosane	338	C24H50	000646-31-1	72
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
5	Octacosane	394	C28H58	000630-02-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

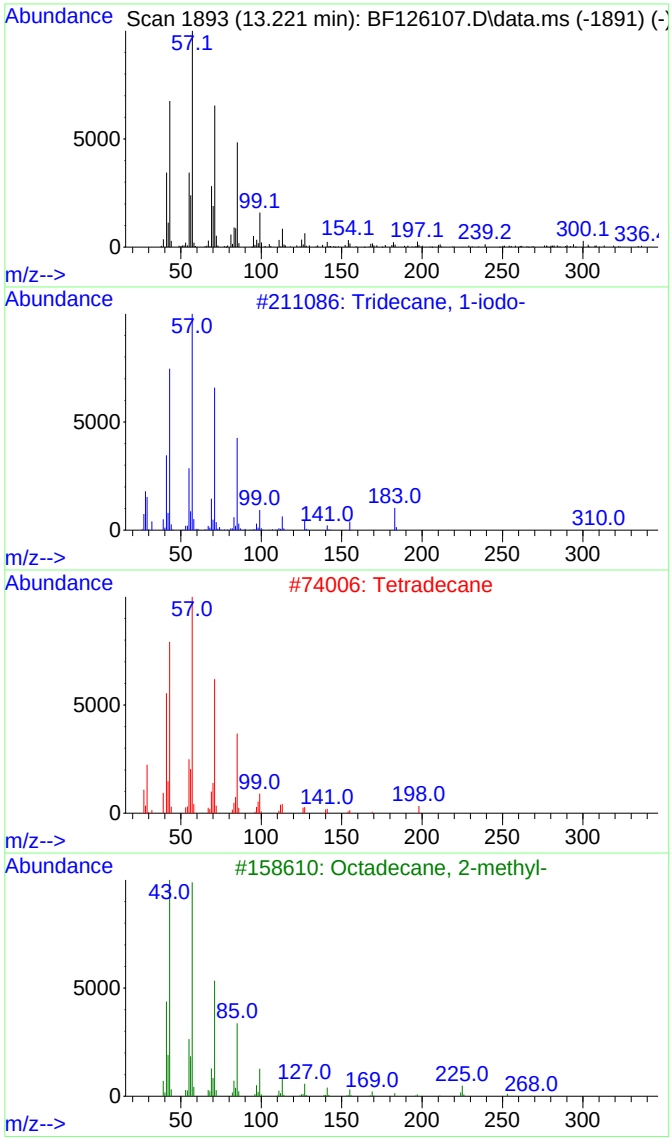
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

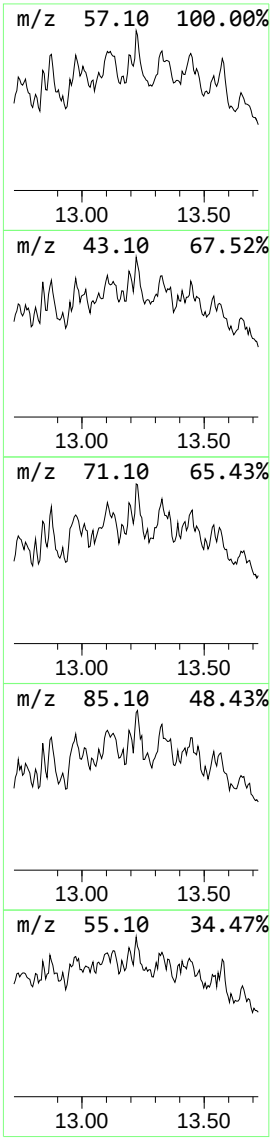
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	11.26 ng	583316	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	Tetradecane	198	C14H30	000629-59-4	87
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	86
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

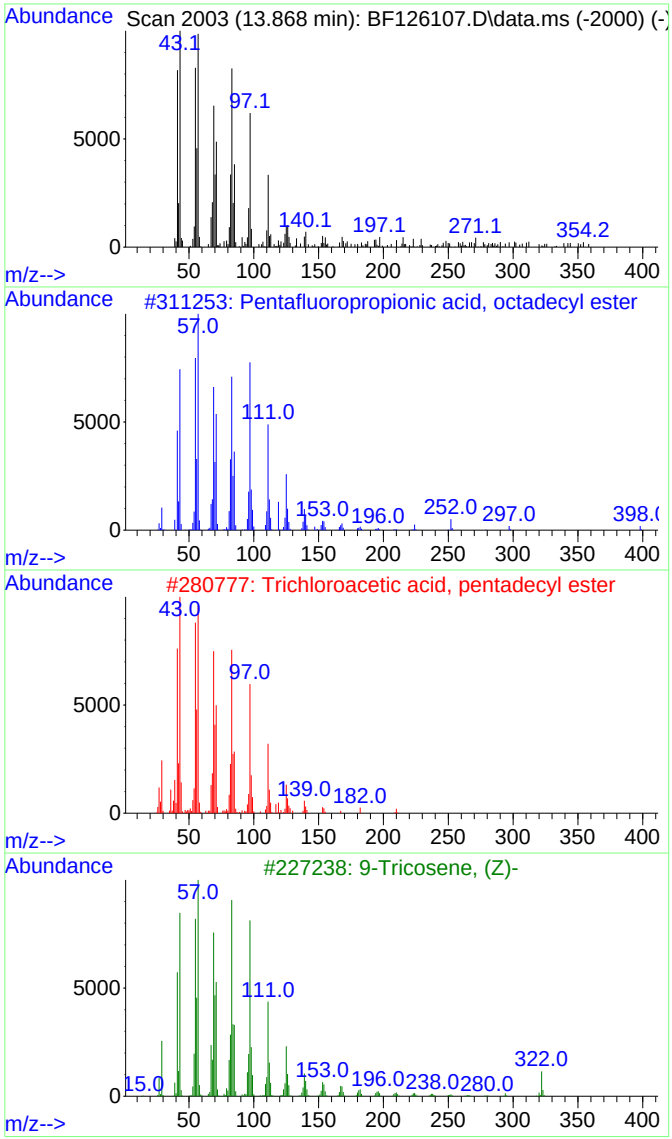
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

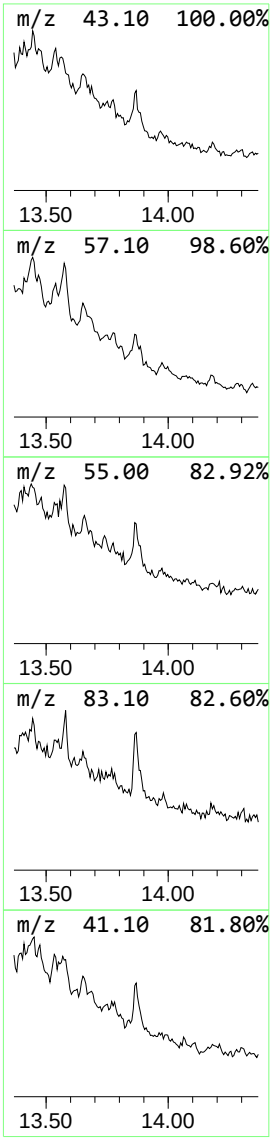
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	15.85 ng	821256	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	87
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

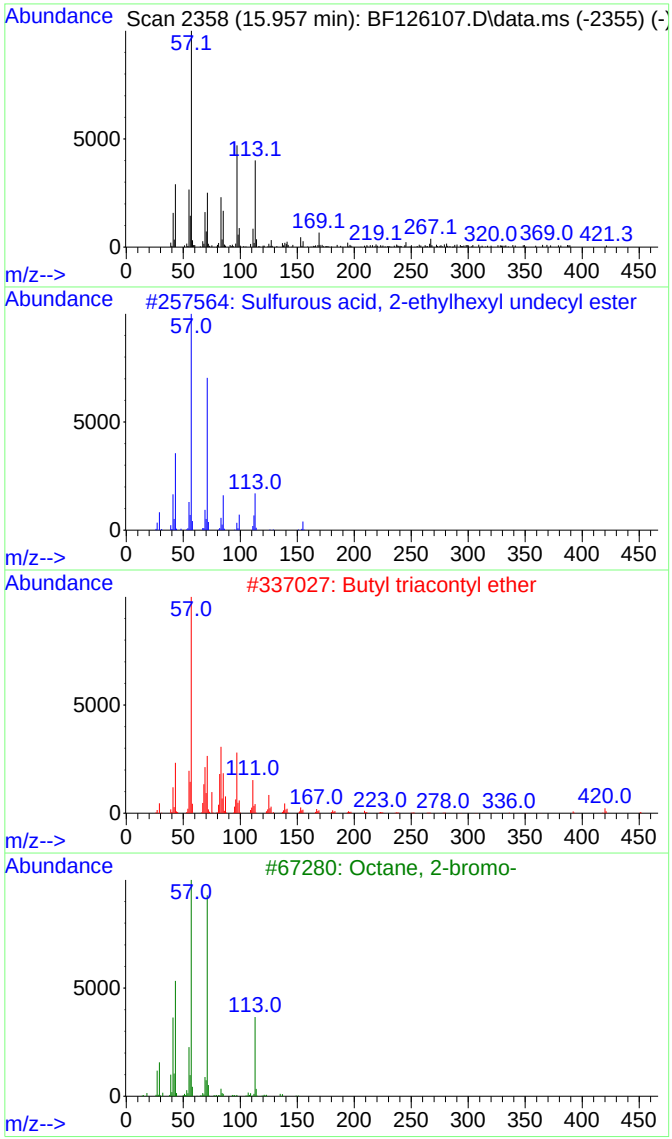
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

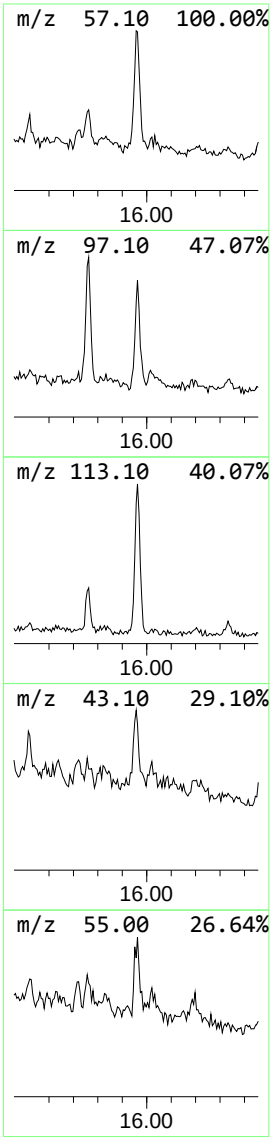
****

Peak Number 20 unknown15.957 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	9.14 ng	343282	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	38
2	Butyl triacontyl ether	495	C34H70O	1000406-41-2	37
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	32
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126107.D
Acq On : 10 Nov 2021 14:56
Operator : JU/CG
Sample : M4595-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CMC-ICS-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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...	2.204	34.0	ng	1914450	1	6.851	1126250	20.0
3-Hexen-2-one	4.469	62.7	ng	3530990	1	6.851	1126250	20.0
2-Pentanone, 4-...	5.093	86.9	ng	4892140	1	6.851	1126250	20.0
Ethanol, 1-(2-b...	8.039	8.8	ng	592516	2	8.133	1345200	20.0
2,4,4,6,6,8,8-H...	10.945	4.0	ng	233492	4	11.374	1169530	20.0
Hexadecane, 2,6...	10.986	4.2	ng	243449	4	11.374	1169530	20.0
Heneicosane	11.269	5.6	ng	325435	4	11.374	1169530	20.0
Nonadecane, 2-m...	11.557	5.0	ng	292428	4	11.374	1169530	20.0
Sulfurous acid,...	11.680	9.4	ng	551348	4	11.374	1169530	20.0
1-Dodecanol, 2-...	11.833	8.1	ng	476225	4	11.374	1169530	20.0
Heptadecane, 2-...	11.969	9.4	ng	551371	4	11.374	1169530	20.0
Tetradecane	12.080	7.6	ng	443570	4	11.374	1169530	20.0
Octacosane	12.233	5.5	ng	321210	4	11.374	1169530	20.0
3,5-Dimethyldod...	12.357	9.2	ng	539982	4	11.374	1169530	20.0
1,5-Dihydroxy-6...	12.398	4.8	ng	283148	4	11.374	1169530	20.0
Tetracosane	12.469	8.4	ng	492491	4	11.374	1169530	20.0
Tetratetracontane	12.874	11.5	ng	594791	5	14.015	1035970	20.0
Tridecane, 1-iodo-	13.221	11.3	ng	583316	5	14.015	1035970	20.0
Pentafluoroprop...	13.868	15.9	ng	821256	5	14.015	1035970	20.0
unknown15.957	15.957	9.1	ng	343282	6	15.480	750758	20.0