LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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: BF126234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	493	496	502	rBV	279005	274827	8.38%	1.038%
2	5.416	562	566	569	rBV	1298953	1107119	33.78%	4.180%
3	6.428	734	738	749	rBV	1257305	1104533	33.70%	4.171%
4	6.816	800	804	807	rBV	1790586	1446139	44.12%	5.460%
5	7.369	894	898	902	rBV	838285	700306	21.37%	2.644%
6	8.098	1018	1022	1025	rBV	2422545	1918754	58.54%	7.245%
7	9.175	1201	1205	1208	rBV	1444448	1133846	34.59%	4.281%
8	9.263	1217	1220	1224	rVB	72731	58707	1.79%	0.222%
9	9.516	1256	1263	1265	rBV6	25484	38396	1.17%	0.145%
10	9.581	1269	1274	1276	rBV4	29479	41017	1.25%	0.155%
11	9.792	1308	1310	1315	rVB	103918	76094	2.32%	0.287%
12	9.851	1315	1320	1324	rBV	2131624	1769373	53.98%	6.681%
13	10.292	1392	1395	1398	rVB	116493	86381	2.64%	0.326%
14	10.510	1428	1432	1438	rVB	45094	56890	1.74%	0.215%
15	10.633	1450	1453	1458	rBV	568822	460983	14.06%	1.741%
16	10.763	1473	1475	1485	rBV	143047	152677	4.66%	0.576%
17	11.210	1549	1551	1554	rBV	96471	89863	2.74%	0.339%
18	11.245	1554	1557	1561	rVB2	42690	46394	1.42%	0.175%
19	11.333	1569	1572	1575	rBV	1543226	1318447	40.22%	4.978%
20	11.357	1575	1576	1579	rVB	214268	119967	3.66%	0.453%
21	11.639	1621	1624	1626	rBV	91108	80262	2.45%	0.303%
22	11.663	1626	1628	1631	rVB2	106028	79278	2.42%	0.299%
23	11.739	1637	1641	1644	rBV	2183425	1695723	51.73%	6.403%
24	11.839	1654	1658	1660	rBV	40435	41249	1.26%	0.156%
25	11.863	1660	1662	1666	rVB	93420	72864	2.22%	0.275%
26	11.945	1672	1676	1679	rBV2	59399	65790	2.01%	0.248%
27	12.045	1690	1693	1702	rVB2	67806	82993	2.53%	0.313%
28	12.145	1702	1710	1718	rBV6	37051	79097	2.41%	0.299%
29	12.386	1744	1751	1754	rBV4	55510	80019	2.44%	0.302%
30	12.427	1754	1758	1759	rVV	3461914	3216732	98.14%	12.146%
31	12.445	1759	1761	1768	rVV2	3416127	3277726	100.00%	12.376%
32	12.527	1772	1775	1781	rBV2	643398	807635	24.64%	3.050%
33	12.574	1781	1783	1787	rVV3	45195	41868	1.28%	0.158%
34	12.774	1811	1817	1820	rBV	283227	322258	9.83%	1.217%
35	12.921	1838	1842	1845	rVB	762107	676651	20.64%	2.555%
36	13.092	1866	1871	1878	rBV2	89122	153939	4.70%	0.581%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

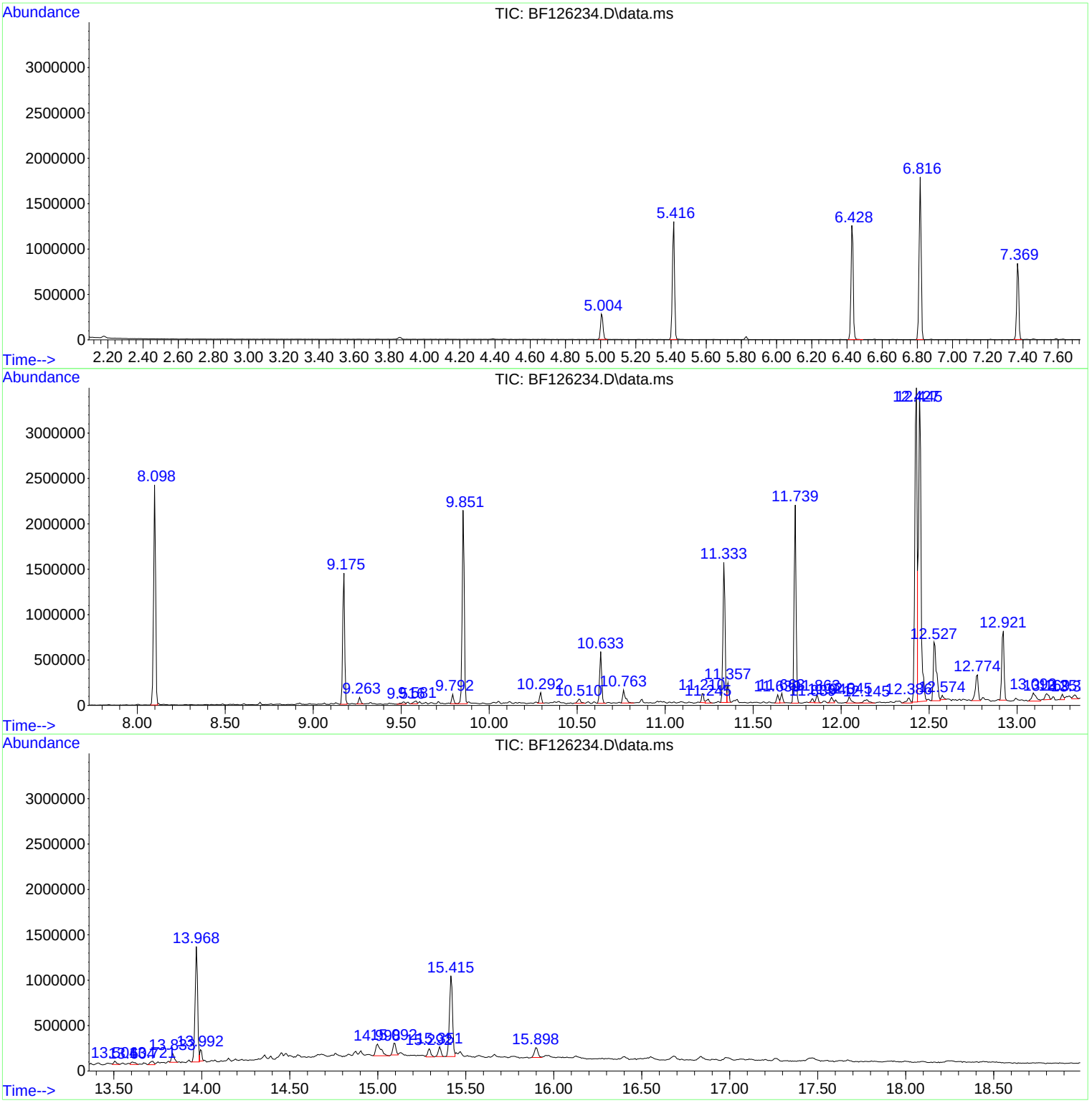
37	13.169	1881	1884	1888	rVV3	63700	93927	2.87%	0.355%
38	13.257	1896	1899	1901	rBV	60605	54875	1.67%	0.207%
39	13.327	1908	1911	1915	rVB4	42982	53596	1.64%	0.202%
40	13.504	1939	1941	1946	rVB5	36246	39720	1.21%	0.150%
41	13.604	1956	1958	1964	rVB2	27099	43662	1.33%	0.165%
42	13.721	1973	1978	1980	rBV3	38080	57829	1.76%	0.218%
43	13.833	1994	1997	2002	rVB	98953	108373	3.31%	0.409%
44	13.968	2015	2020	2023	rBV	1271305	1286041	39.24%	4.856%
45	13.992	2023	2024	2027	rVB	123445	92648	2.83%	0.350%
46	14.998	2191	2195	2207	rVB	128188	266961	8.14%	1.008%
47	15.092	2208	2211	2215	rBV2	129896	159164	4.86%	0.601%
48	15.292	2242	2245	2250	rVB	89871	105350	3.21%	0.398%
49	15.351	2252	2255	2259	rVB	106739	111013	3.39%	0.419%
50	15.415	2261	2266	2270	rBV	888849	1078618	32.91%	4.073%
51	15.898	2344	2348	2354	rBV	109298	157557	4.81%	0.595%

Sum of corrected areas: 26484131

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

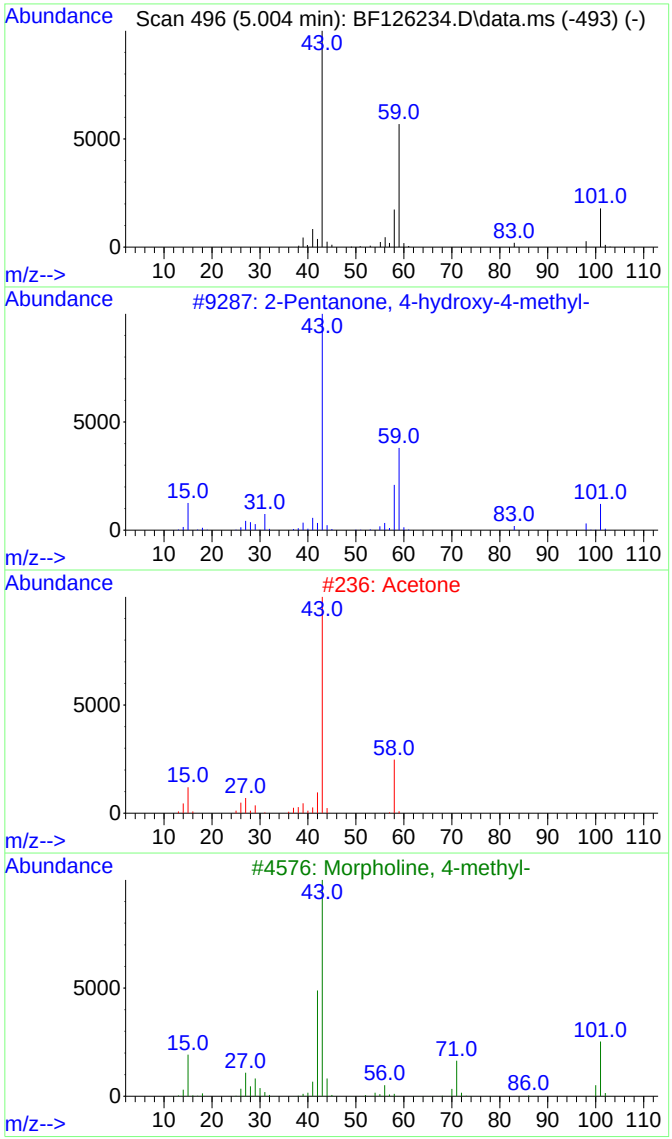
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

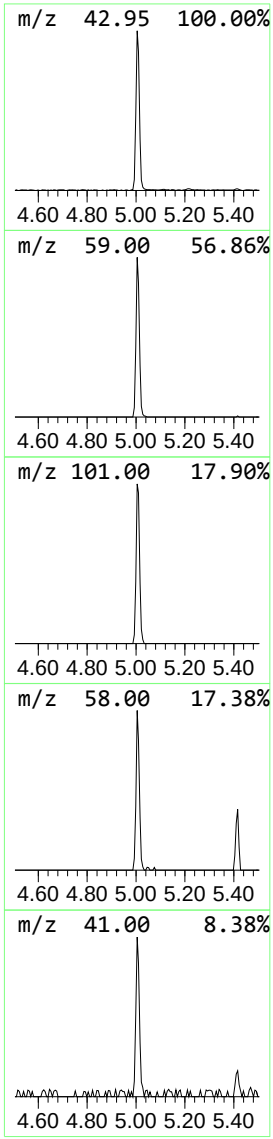
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	3.80 ng	274827	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	Acetone	58	C3H6O	000067-64-1	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

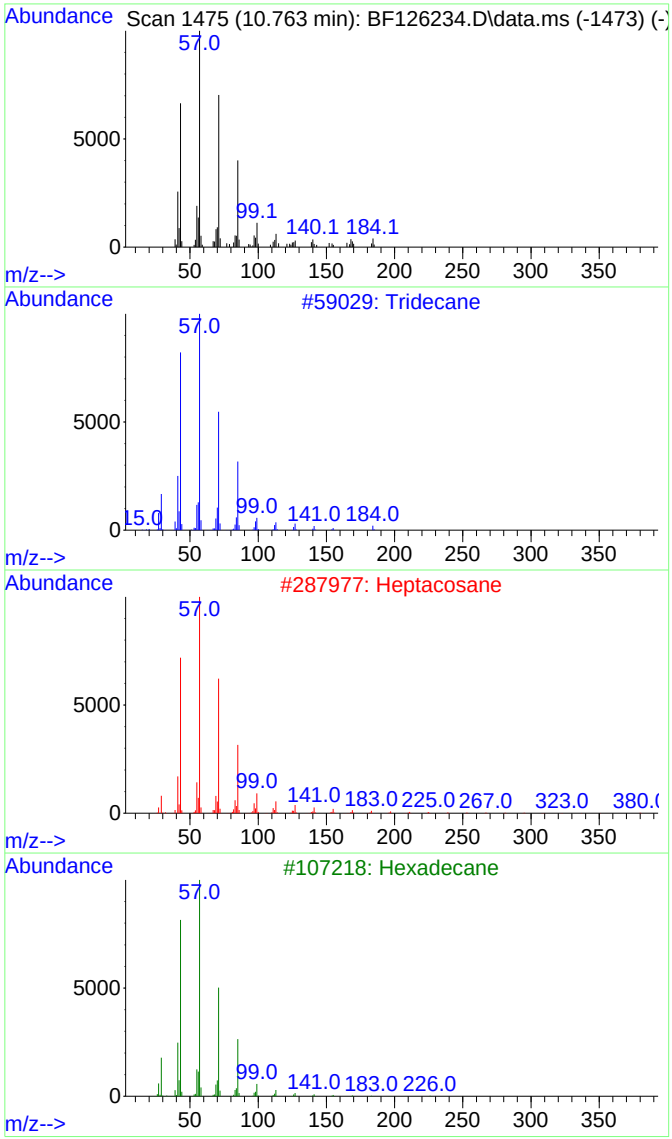
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

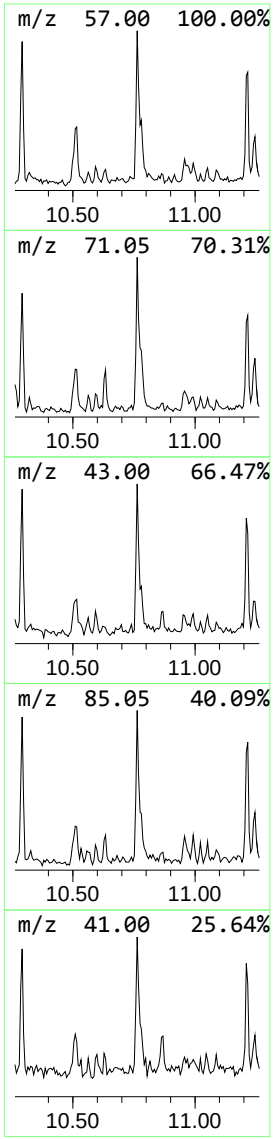
****

Peak Number 2 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	2.32 ng	152677	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5	Heptadecane	240	C17H36	000629-78-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

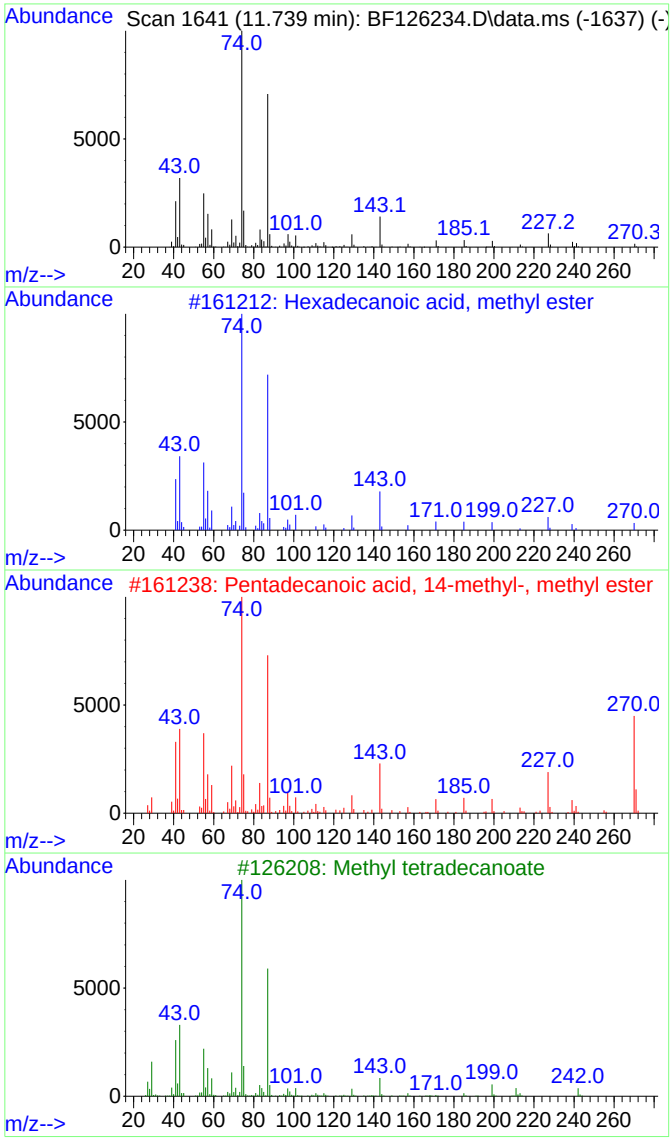
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

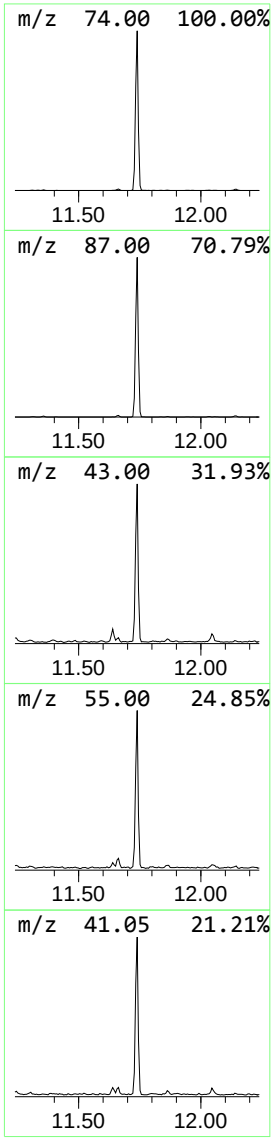
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	25.72 ng	1695720	Phenanthrene-d10	11.333

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	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

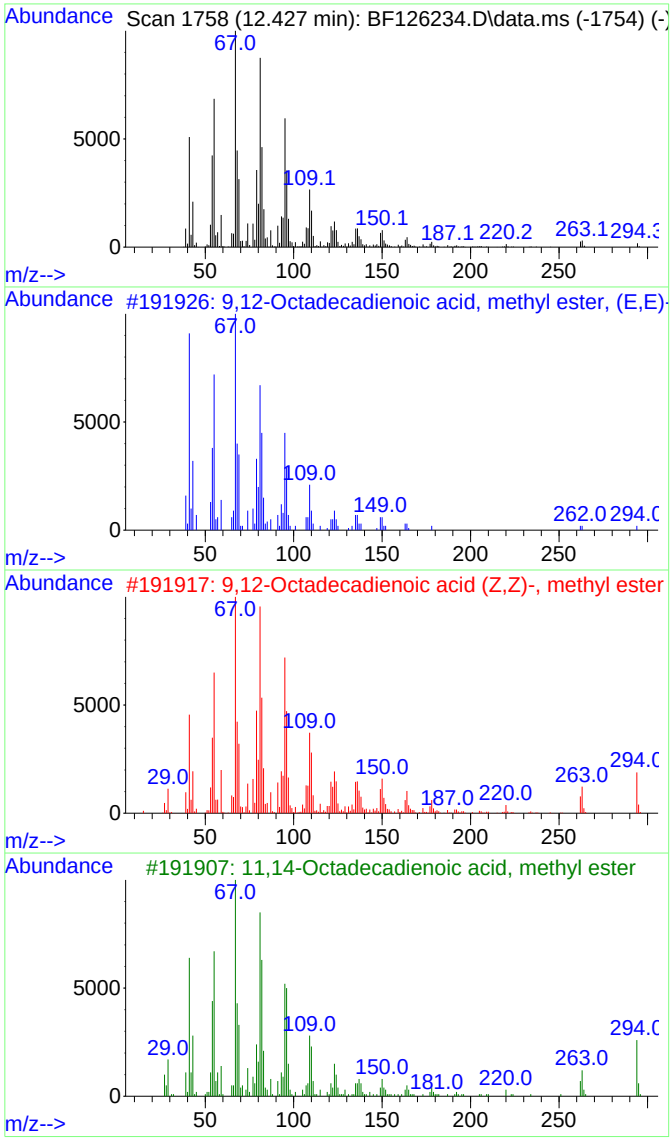
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

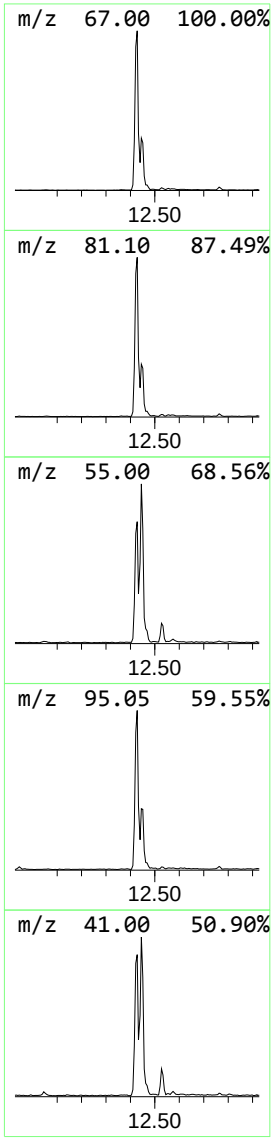
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	48.80 ng	3216730	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

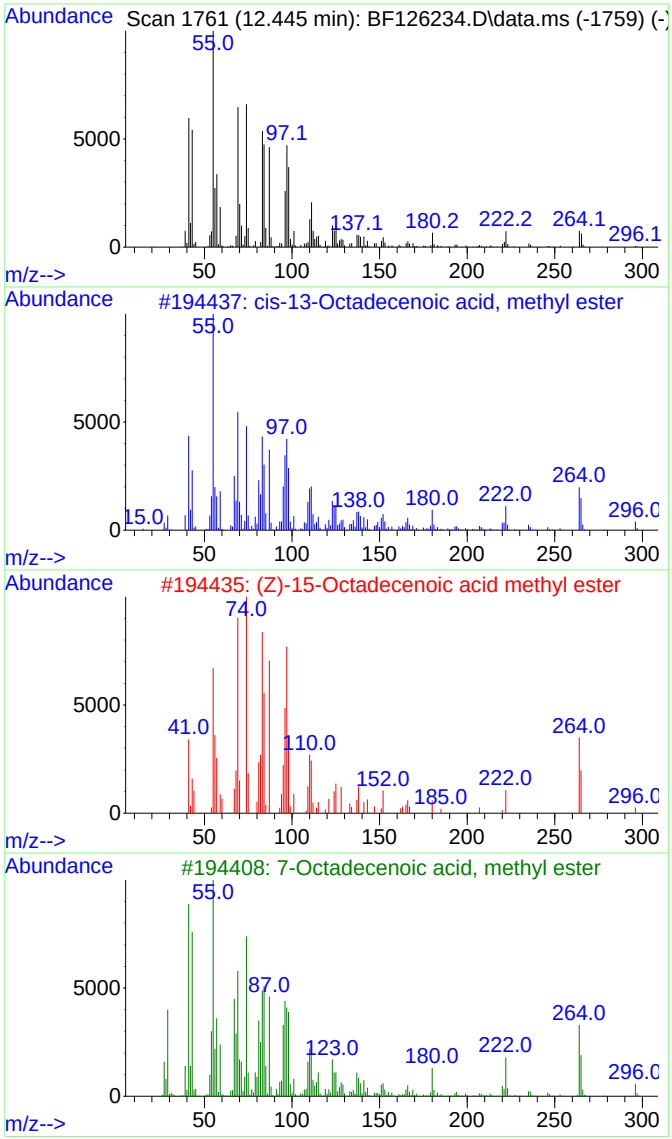
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

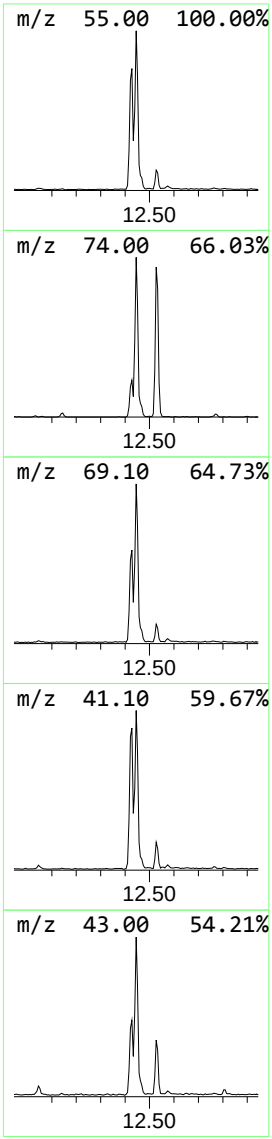
****

Peak Number 5 cis-13-Octadecenoic acid, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	49.72 ng	3277730	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	93
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	91
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	91
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	90
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

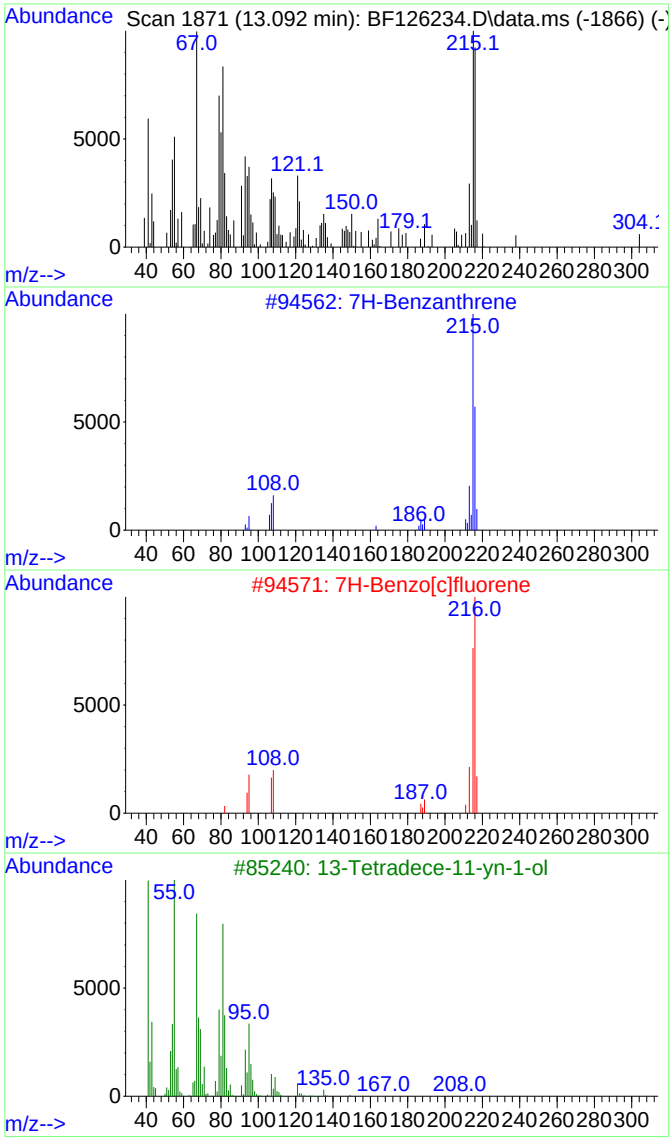
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

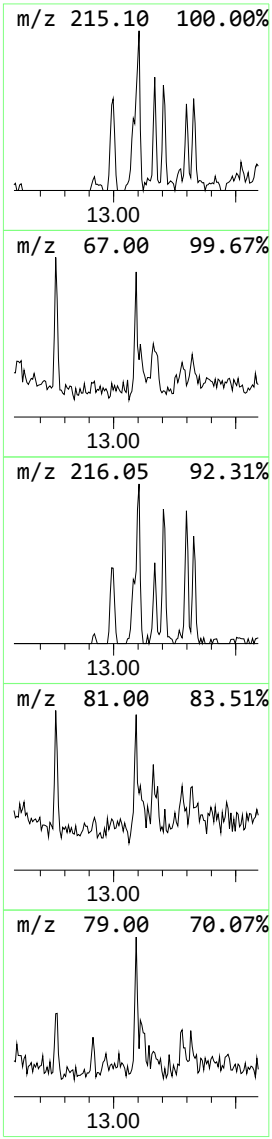
****

Peak Number 6 7H-Benzanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.092	2.39 ng	153939	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benzanthrene	216	C17H12	000199-94-0	52
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	46
3	13-Tetradece-11-yn-1-ol	208	C14H24O	1000131-00-4	38
4	Tricyclo[4.3.1.0(2,5)]decane	136	C10H16	042210-02-6	35
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

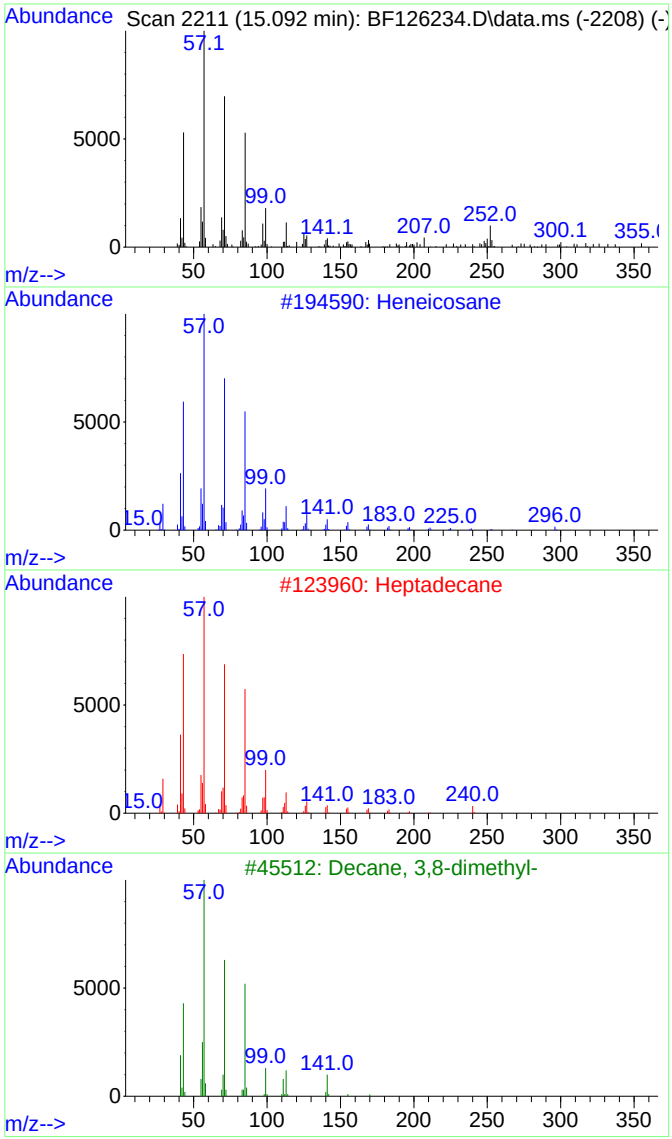
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

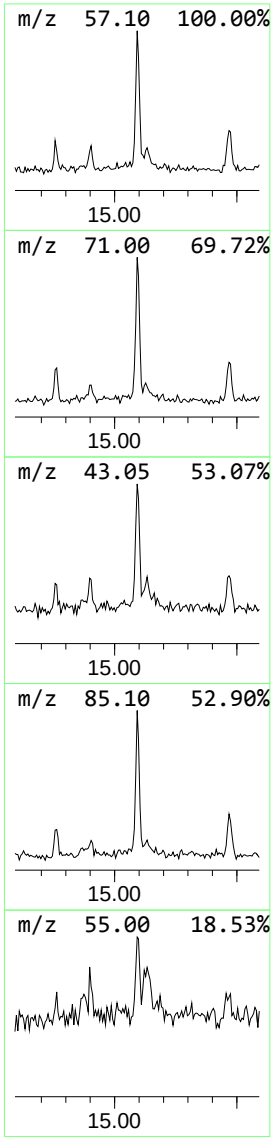
****

Peak Number 7 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.95 ng	159164	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Heptadecane	240	C17H36	000629-78-7	74
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	74
5	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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

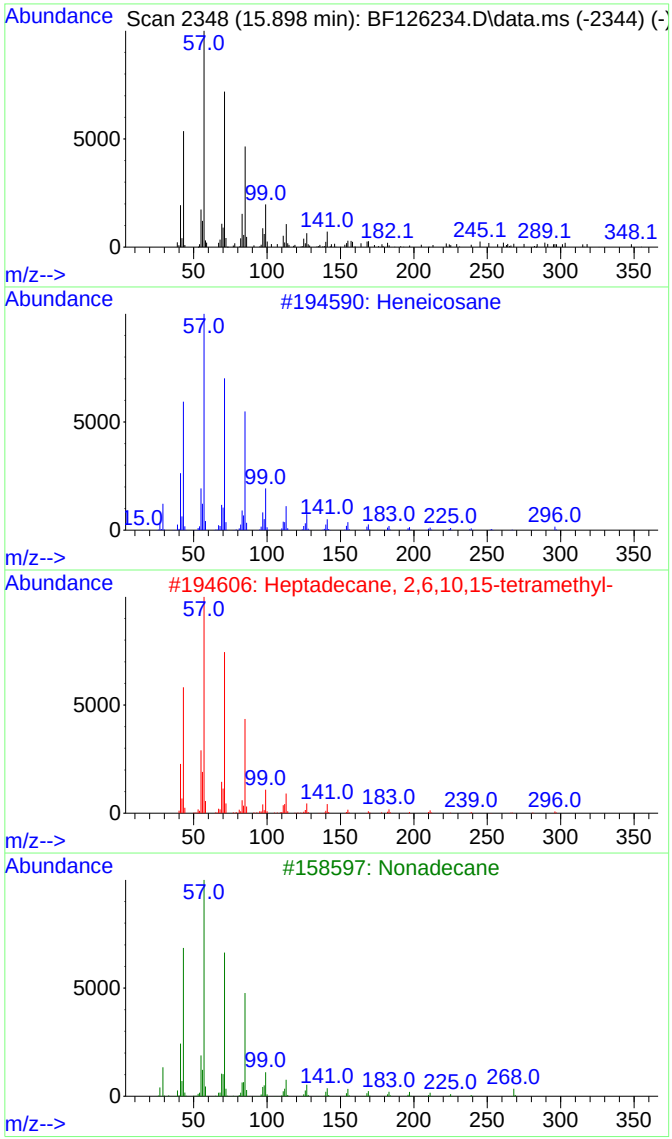
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

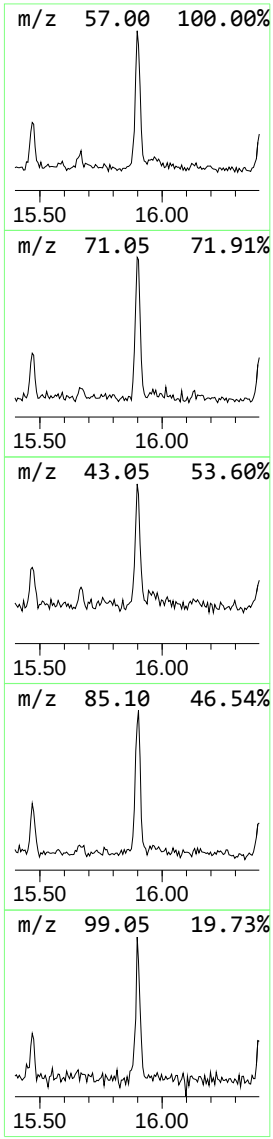
****

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.92 ng	157557	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126234.D
Acq On : 17 Dec 2021 14:35
Operator : JU/CG
Sample : M5030-01 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

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
2-Pentanone, 4-...	5.004	3.8	ng	274827	1	6.816	1446140	20.0
Tridecane	10.763	2.3	ng	152677	4	11.333	1318450	20.0
Hexadecanoic ac...	11.739	25.7	ng	1695720	4	11.333	1318450	20.0
9,12-Octadecadi...	12.427	48.8	ng	3216730	4	11.333	1318450	20.0
cis-13-Octadece...	12.445	49.7	ng	3277730	4	11.333	1318450	20.0
7H-Benzanthrene	13.092	2.4	ng	153939	5	13.969	1286040	20.0
Heptadecane	15.092	3.0	ng	159164	6	15.415	1078620	20.0
Heneicosane	15.898	2.9	ng	157557	6	15.415	1078620	20.0