LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PSC164718

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: BF126369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.540	74	77	85	rBV	34748	49163	2.38%	0.309%
2	3.234	192	195	205	rBV2	22186	51647	2.50%	0.325%
3	5.010	493	497	509	rVB	76233	98864	4.78%	0.622%
4	5.422	562	567	570	rBV	1999380	2032436	98.24%	12.786%
5	6.434	734	739	753	rBV	1978391	2068813	100.00%	13.014%
6	6.810	799	803	806	rBV	744092	613215	29.64%	3.858%
7	7.369	893	898	901	rBV	1474444	1295734	62.63%	8.151%
8	8.092	1016	1021	1026	rBV	895232	791234	38.25%	4.977%
9	8.522	1090	1094	1096	rBV	23991	21828	1.06%	0.137%
10	8.686	1119	1122	1127	rVB	81609	72155	3.49%	0.454%
11	9.169	1200	1204	1207	rBV	2134056	1768110	85.46%	11.123%
12	9.257	1215	1219	1224	rBV	115533	103813	5.02%	0.653%
13	9.575	1268	1273	1275	rBV2	48832	55104	2.66%	0.347%
14	9.786	1306	1309	1313	rVB	111545	99094	4.79%	0.623%
15	9.845	1313	1319	1323	rBV	827018	690097	33.36%	4.341%
16	10.010	1343	1347	1351	rBV5	13561	20768	1.00%	0.131%
17	10.104	1359	1363	1367	rVB3	16909	22236	1.07%	0.140%
18	10.263	1386	1390	1391	rBV2	26170	27555	1.33%	0.173%
19	10.280	1391	1393	1396	rVB	97106	80291	3.88%	0.505%
20	10.504	1425	1431	1434	rBV	42254	46716	2.26%	0.294%
21	10.633	1449	1453	1457	rBV	898744	854448	41.30%	5.375%
22	10.757	1471	1474	1479	rBV	103586	117076	5.66%	0.736%
23	11.204	1547	1550	1553	rBV	71704	55912	2.70%	0.352%
24	11.233	1553	1555	1560	rVB2	30256	29888	1.44%	0.188%
25	11.327	1568	1571	1574	rBV	642933	555123	26.83%	3.492%
26	11.351	1574	1575	1578	rVV	88112	60675	2.93%	0.382%
27	11.404	1582	1584	1590	rVB	20817	22788	1.10%	0.143%
28	11.633	1620	1623	1627	rBV	55121	46528	2.25%	0.293%
29	11.863	1659	1662	1665	rBV2	37667	38318	1.85%	0.241%
30	11.945	1671	1676	1678	rBV2	24555	25561	1.24%	0.161%
31	12.039	1689	1692	1695	rBV	44405	33516	1.62%	0.211%
32	12.427	1754	1758	1762	rVB3	33054	32598	1.58%	0.205%
33	12.539	1774	1777	1780	rBV	151827	129889	6.28%	0.817%
34	12.769	1809	1816	1819	rBV	145997	141328	6.83%	0.889%
35	12.916	1837	1841	1845	rVB	1554894	1384058	66.90%	8.707%
36	13.098	1870	1872	1878	rVB2	22556	21128	1.02%	0.133%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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	13.163	1879	1883	1885	rBV2	22112	25606	1.24%	0.161%
38	13.398	1919	1923	1928	rVB3	20174	30031	1.45%	0.189%
39	13.604	1956	1958	1964	rVB3	16469	24326	1.18%	0.153%
40	13.886	1999	2006	2014	rBV8	46217	135208	6.54%	0.851%
41	13.968	2015	2020	2023	rVV	709811	744695	36.00%	4.685%
42	13.992	2023	2024	2027	rVB	87283	53284	2.58%	0.335%
43	14.663	2134	2138	2140	rBV5	17030	25718	1.24%	0.162%
44	14.733	2147	2150	2153	rBV4	25368	33924	1.64%	0.213%
45	14.827	2163	2166	2173	rBV5	21118	35032	1.69%	0.220%
46	14.998	2191	2195	2205	rVB	121264	222714	10.77%	1.401%
47	15.098	2207	2212	2216	rVV3	22526	43646	2.11%	0.275%
48	15.292	2241	2245	2250	rVB	76623	89674	4.33%	0.564%
49	15.351	2251	2255	2262	rBV	79546	101248	4.89%	0.637%
50	15.415	2262	2266	2270	rBV	509561	620854	30.01%	3.906%
51	15.892	2343	2347	2351	rVB3	25861	35712	1.73%	0.225%
52	16.833	2504	2507	2517	rVB2	28990	64241	3.11%	0.404%
53	17.268	2576	2581	2592	rVB3	23448	52647	2.54%	0.331%

Sum of corrected areas: 15896267

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
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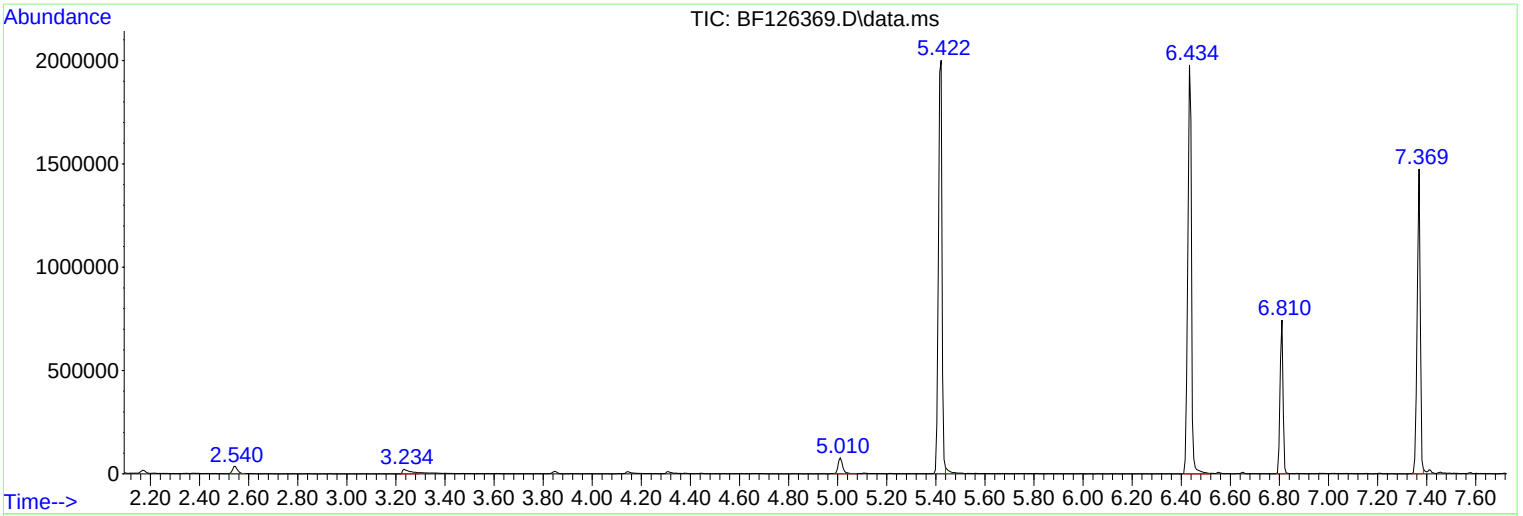
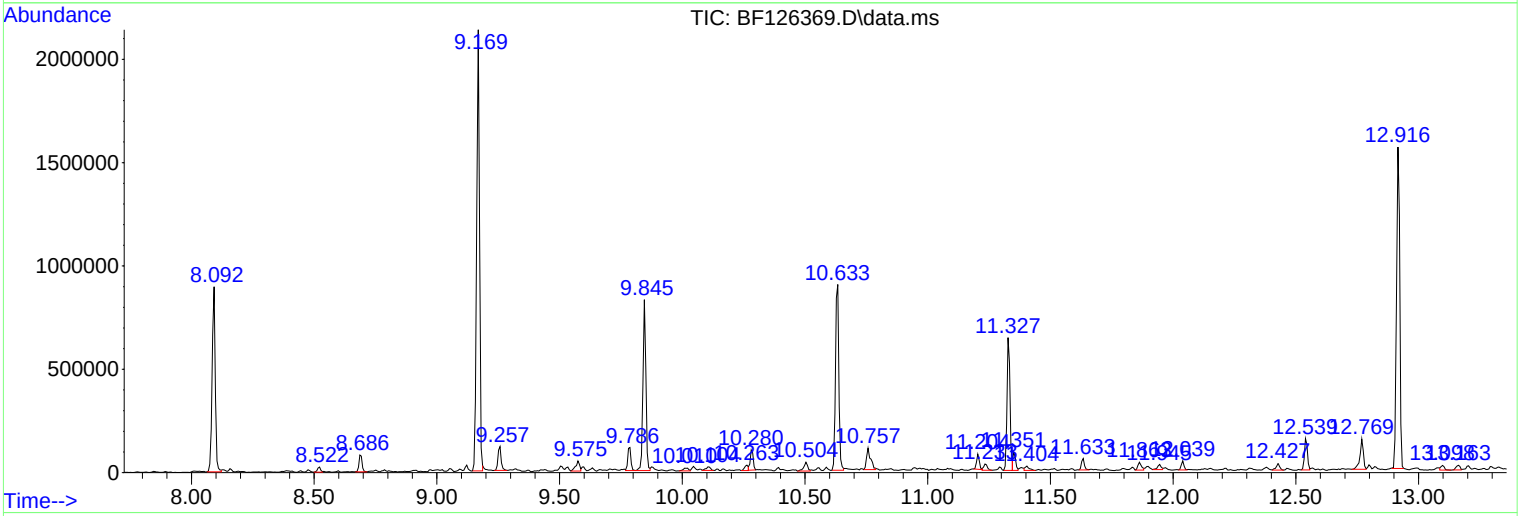
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

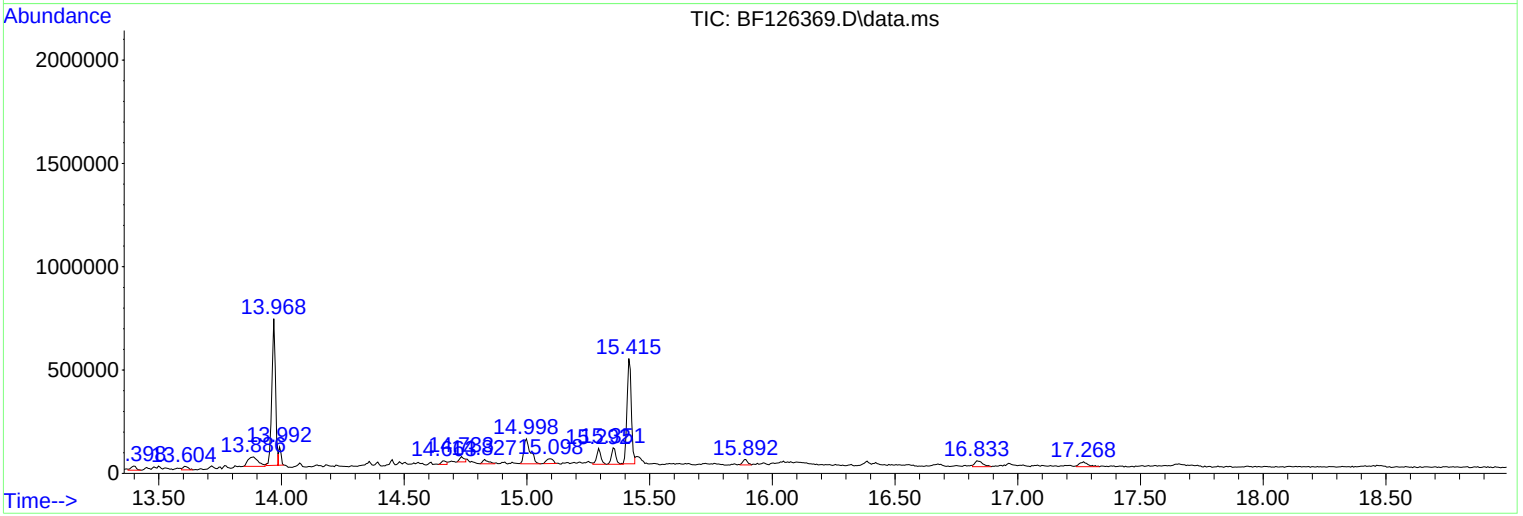
Instrument :
BNA_F
ClientSampleId :
PSC164718

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\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

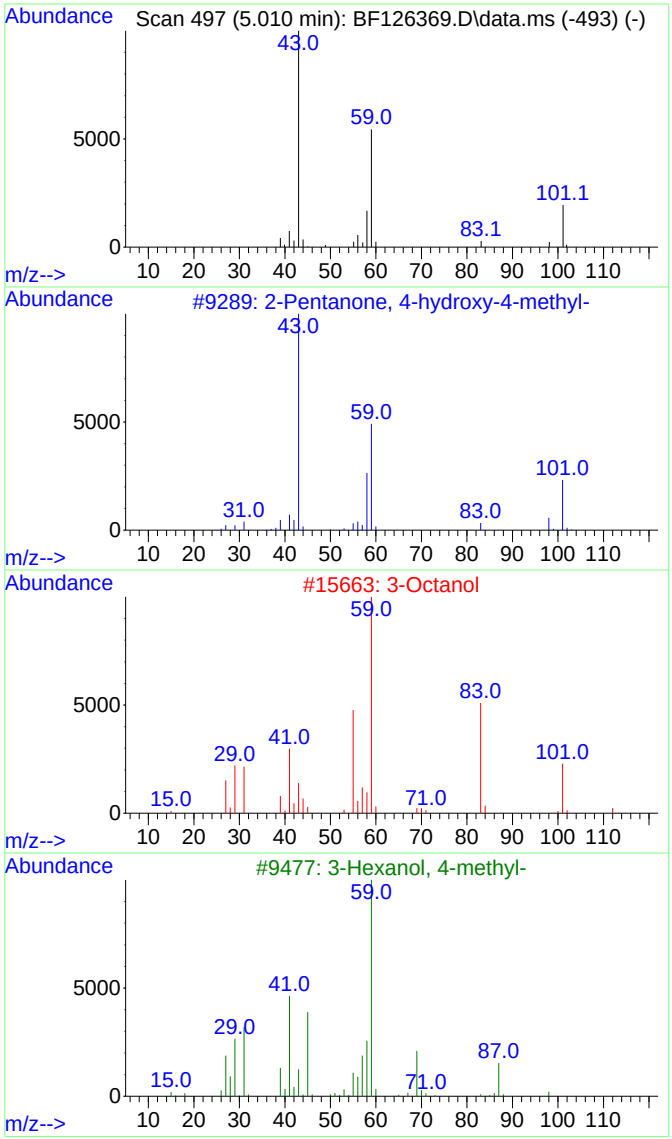
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

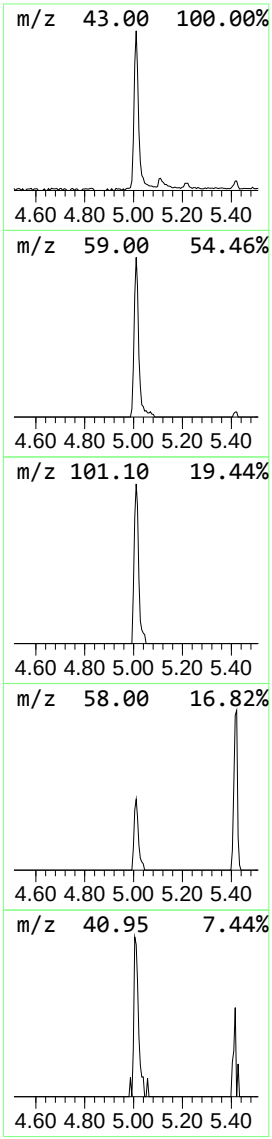
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	3.22 ng	98864	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Octanol	130	C8H18O	000589-98-0	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
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Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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

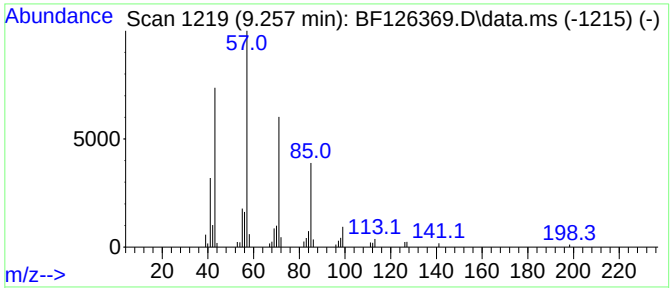
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

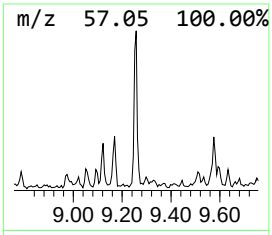
****

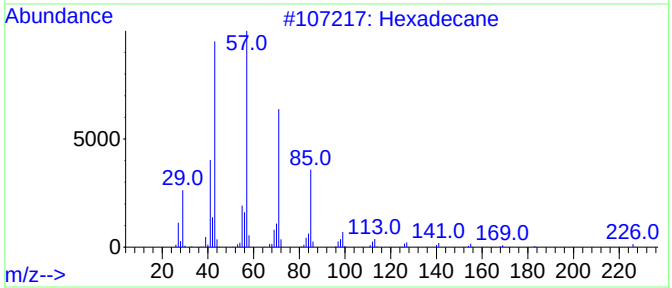
Peak Number 2 Hexadecane Concentration Rank 4

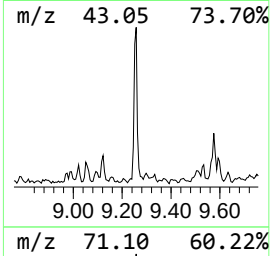
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	3.01 ng	103813	Acenaphthene-d10	9.845

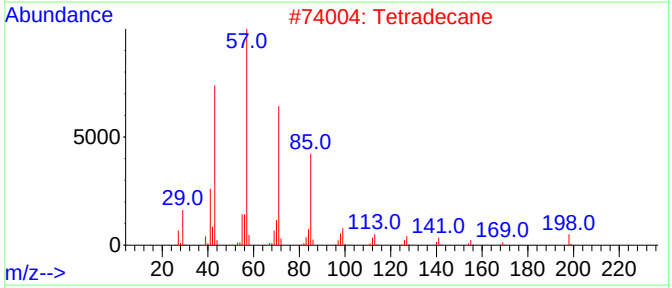
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83

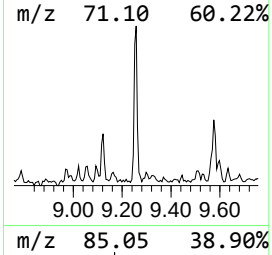


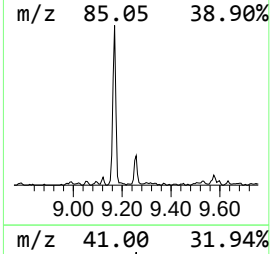


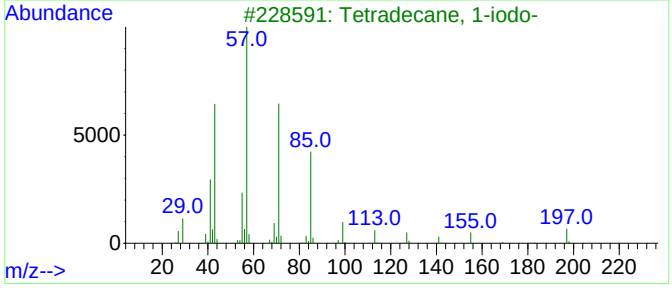


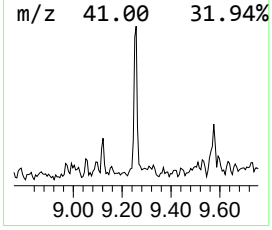












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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

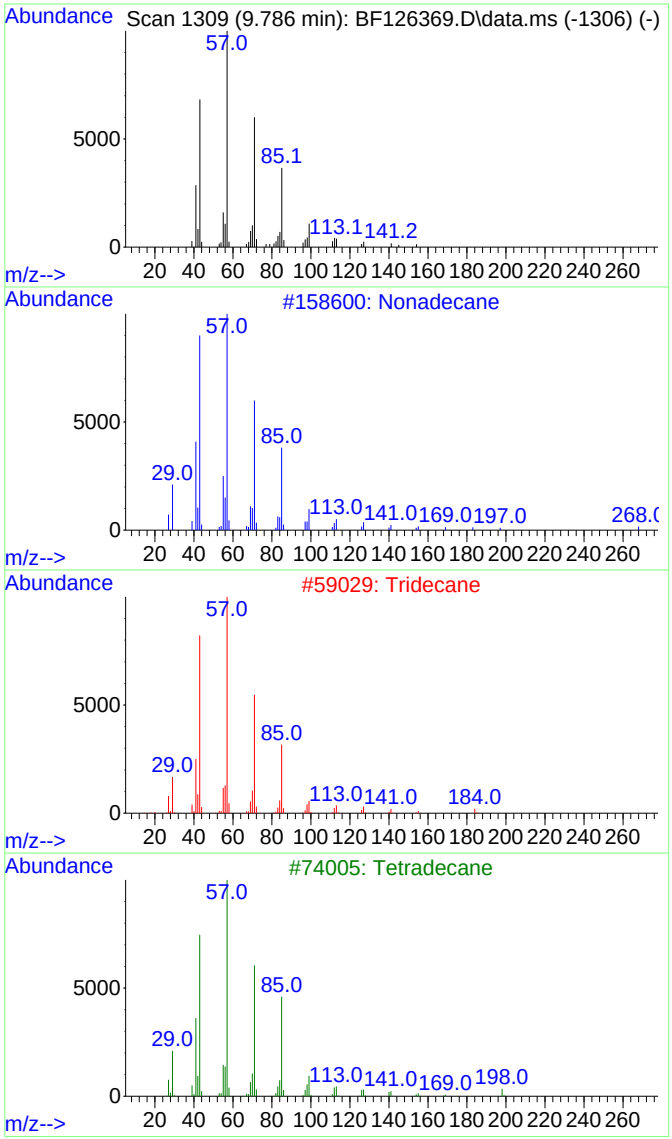
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

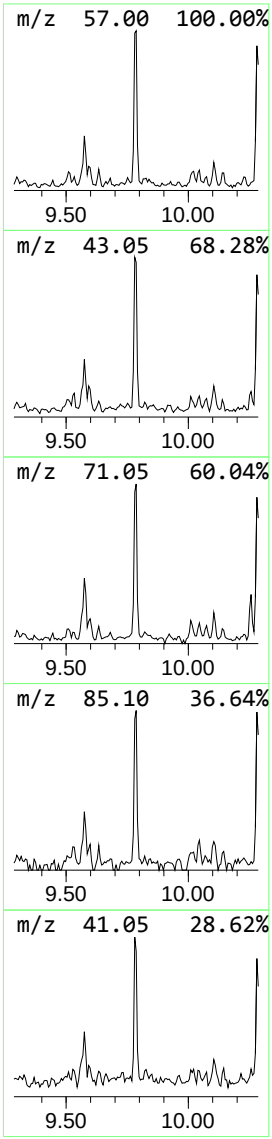
****

Peak Number 3 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.786	2.87 ng	99094	Acenaphthene-d10	9.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tridecane	184	C13H28	000629-50-5	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
5	Pentadecane	212	C15H32	000629-62-9	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

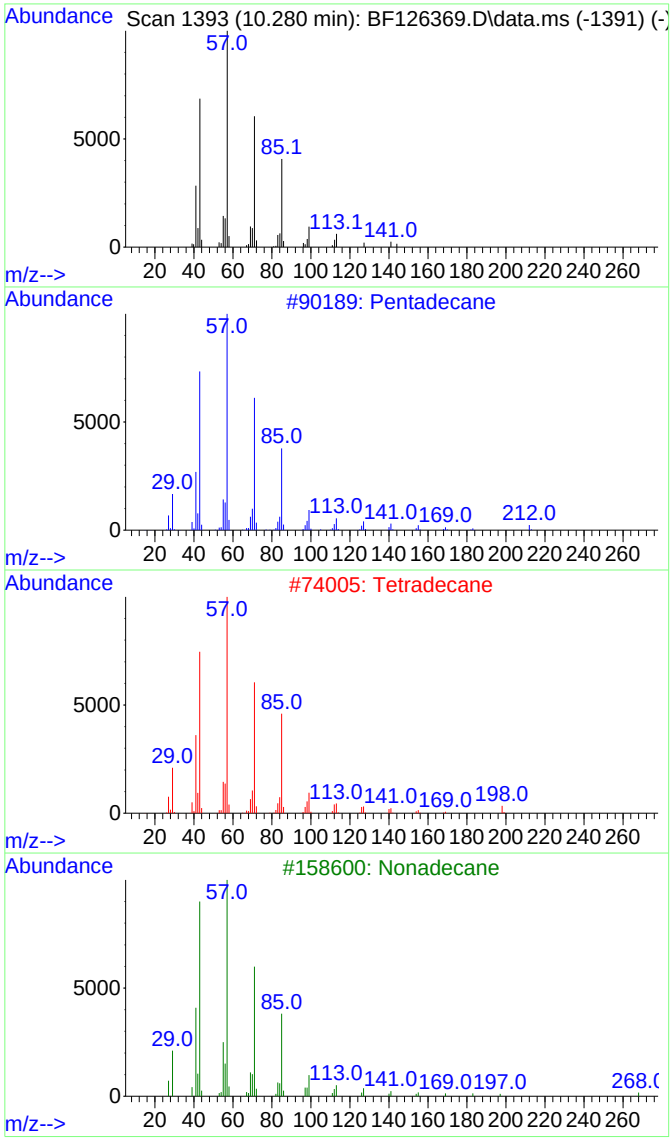
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

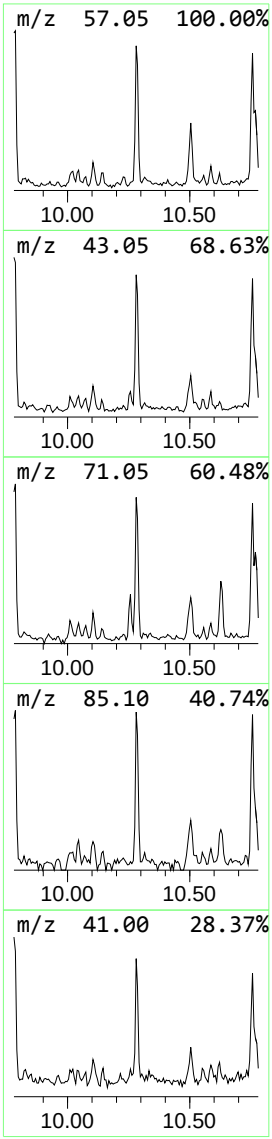
****

Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.281	2.33 ng	80291	Acenaphthene-d10	9.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Nonadecane	268	C19H40	000629-92-5	83
4	Heneicosane	296	C21H44	000629-94-7	80
5	Heptacosane	380	C27H56	000593-49-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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

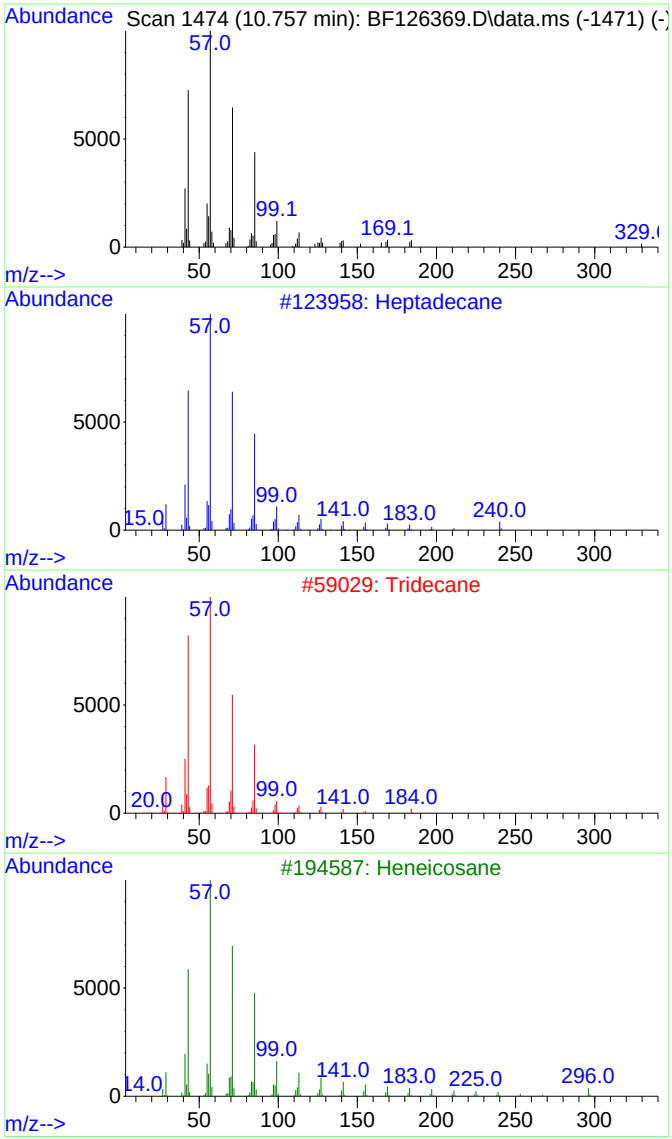
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

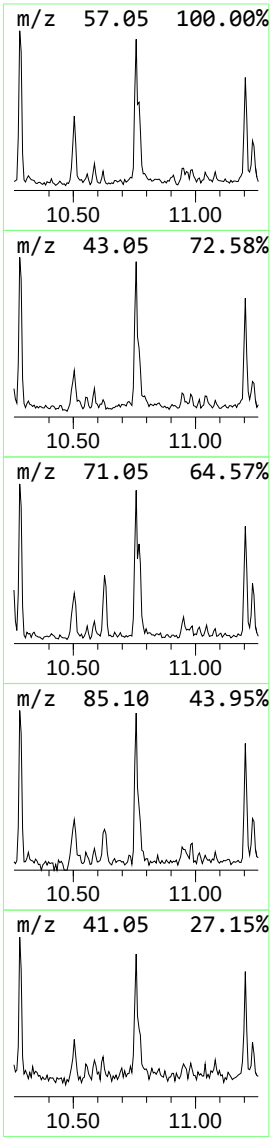
****

Peak Number 5 Heptadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	4.22 ng	117076	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tridecane	184	C13H28	000629-50-5	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

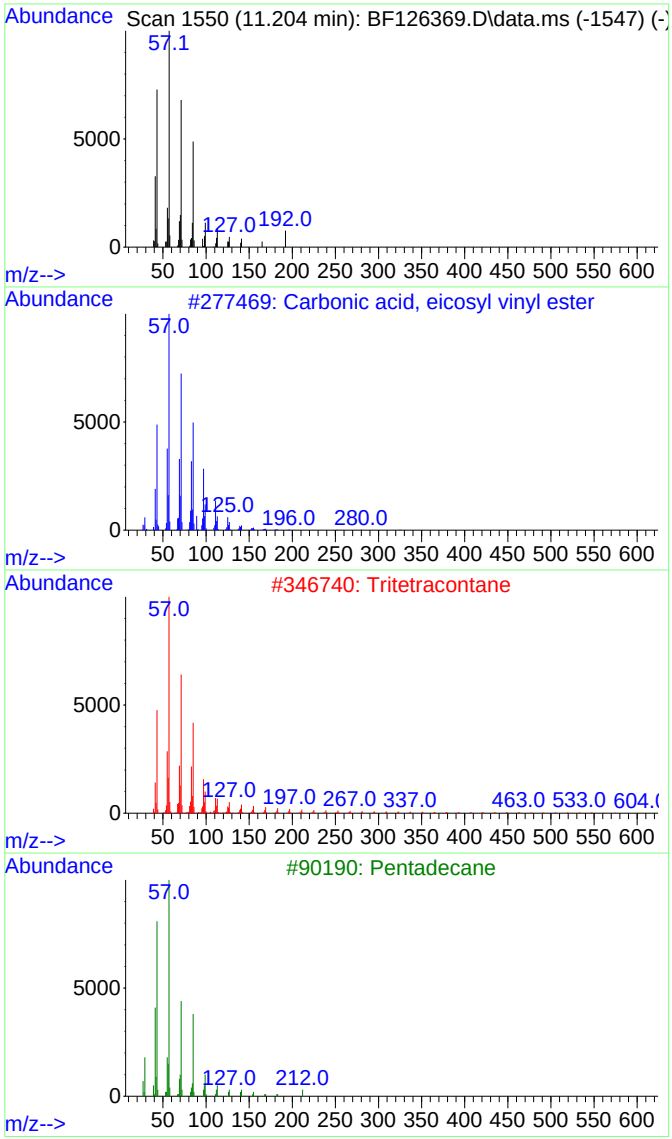
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

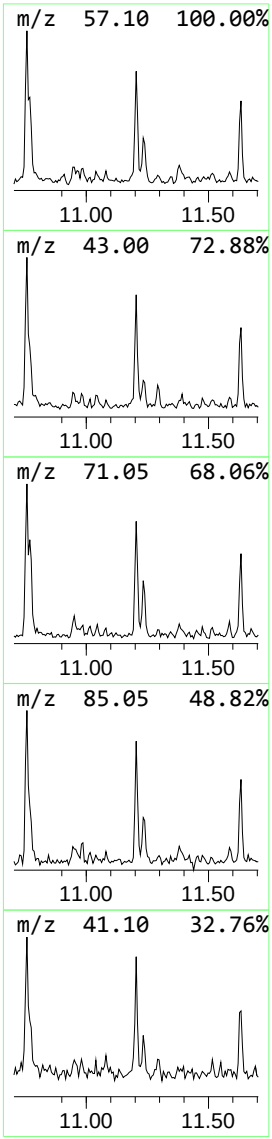
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Carbonic acid, eicosyl viny... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.204	2.01 ng	55912	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2	Tritetracontane	605	C43H88	007098-21-7	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetradecane	198	C14H30	000629-59-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

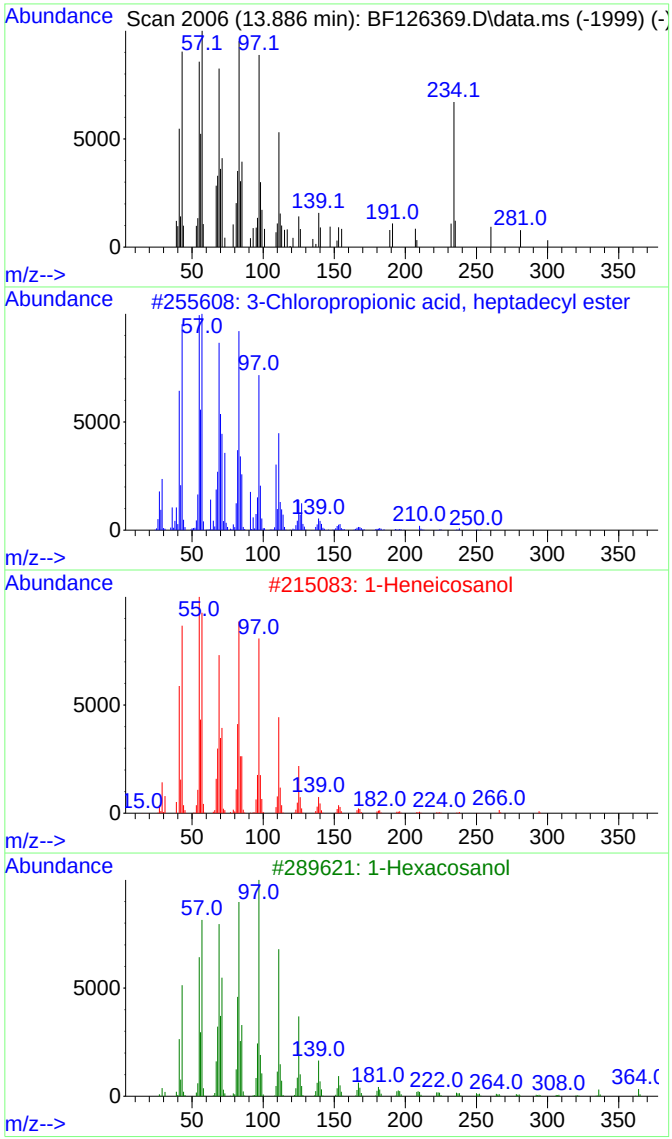
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

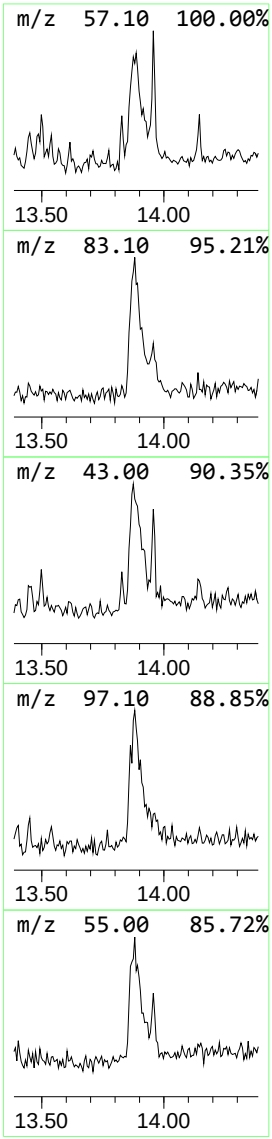
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.63 ng	135208	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
2	1-Heneicosanol	312	C21H44O	015594-90-8	74
3	1-Hexacosanol	382	C26H54O	000506-52-5	68
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	68
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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

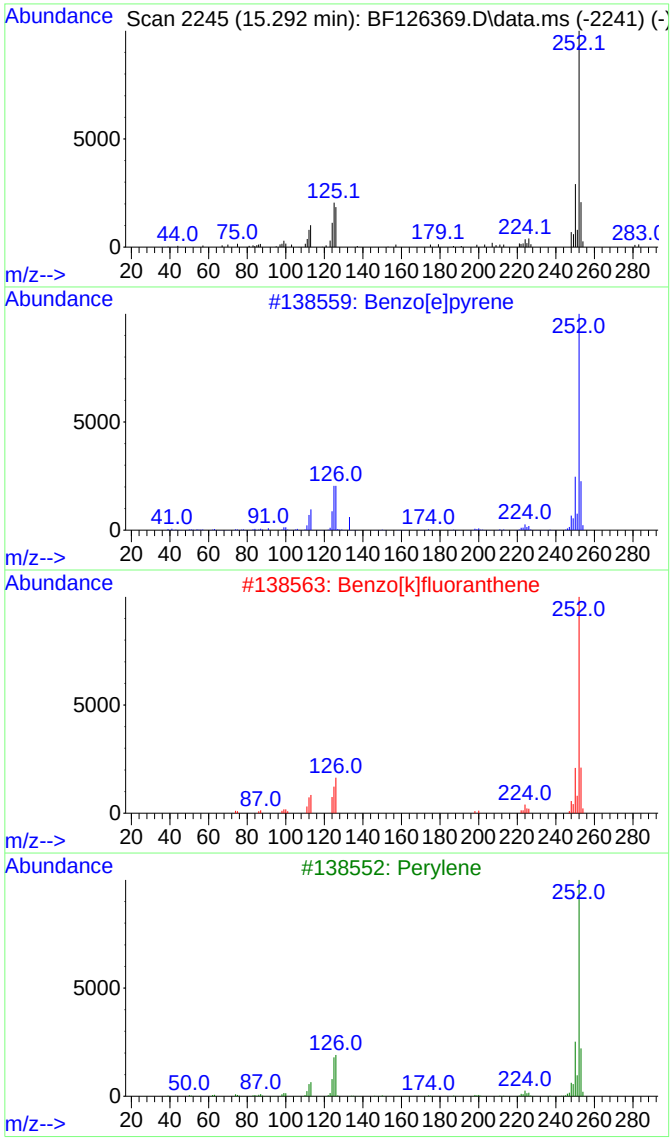
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

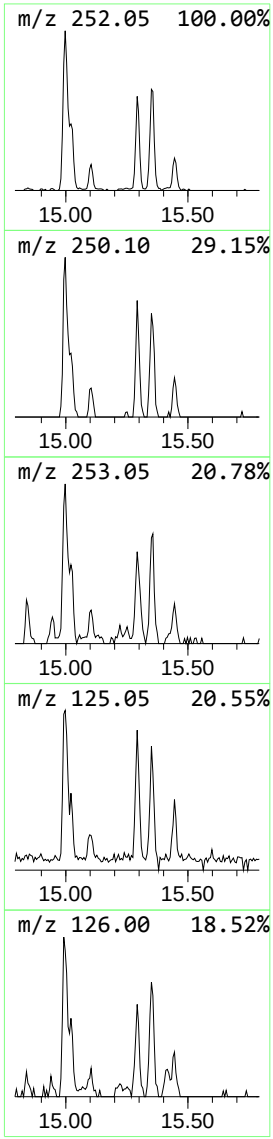
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	2.89 ng	89674	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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

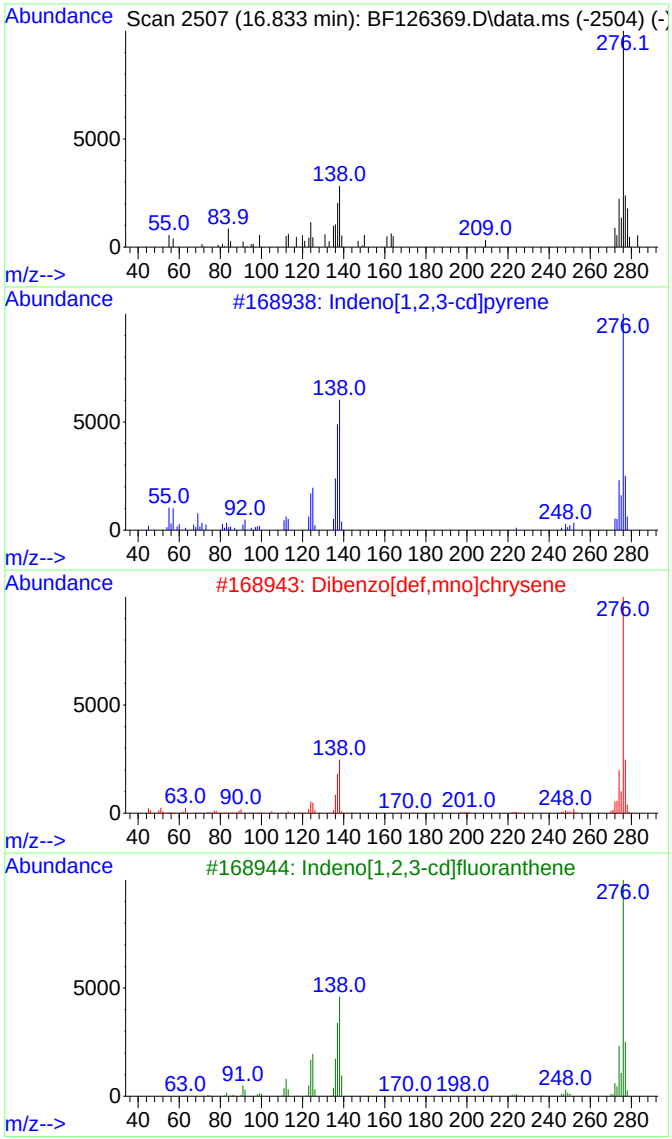
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

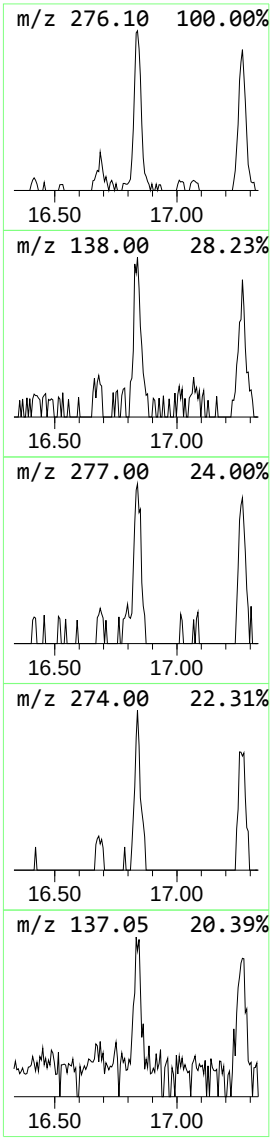
****

Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.833	2.07 ng	64241	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	91
2	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	87
3	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	81
4	Benzo[ghi]perylene	276	C22H12	000191-24-2	81
5	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126369.D
Acq On : 27 Dec 2021 22:15
Operator : JU/CG
Sample : M5230-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC164718

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-...	5.010	3.2	ng	98864	1	6.810	613215	20.0
Hexadecane	9.257	3.0	ng	103813	3	9.845	690097	20.0
Nonadecane	9.786	2.9	ng	99094	3	9.845	690097	20.0
Pentadecane	10.281	2.3	ng	80291	3	9.845	690097	20.0
Heptadecane	10.757	4.2	ng	117076	4	11.328	555123	20.0
Carbonic acid, ...	11.204	2.0	ng	55912	4	11.328	555123	20.0
3-Chloropropion...	13.886	3.6	ng	135208	5	13.969	744695	20.0
Benzo[e]pyrene	15.292	2.9	ng	89674	6	15.415	620854	20.0
Dibenzo[def,mno...	16.833	2.1	ng	64241	6	15.415	620854	20.0