LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052024\
Data File : BF137963.D
Acq On : 20 May 2024 17:08
Operator : CG\JU
Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WCS-TPI

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-BF051424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	15	23	rVB2	48859	115192	3.78%	0.371%
2	2.405	45	54	60	rBV	1685455	2212118	72.63%	7.119%
3	2.522	68	74	81	rBV	27179	35408	1.16%	0.114%
4	3.675	267	270	283	rBV	32506	59727	1.96%	0.192%
5	5.663	603	608	611	rBV	2502057	2255871	74.07%	7.260%
6	6.651	771	776	779	rBV	2367948	2265593	74.39%	7.291%
7	7.040	838	842	845	rBV	1080724	809264	26.57%	2.604%
8	7.598	932	937	940	rBV	1659274	1468790	48.22%	4.727%
9	7.840	974	978	984	rBV	59701	47253	1.55%	0.152%
10	8.322	1056	1060	1063	rBV	1413951	1099510	36.10%	3.538%
11	8.622	1109	1111	1120	rVB	40561	44622	1.47%	0.144%
12	9.398	1238	1243	1246	rBV	3579012	3045742	100.00%	9.802%
13	9.463	1251	1254	1258	rVB	60024	47675	1.57%	0.153%
14	9.734	1292	1300	1303	rBV5	17970	35856	1.18%	0.115%
15	9.939	1331	1335	1338	rBV	35725	36014	1.18%	0.116%
16	9.992	1341	1344	1348	rVB	124952	91762	3.01%	0.295%
17	10.081	1356	1359	1363	rBV	1591752	1280319	42.04%	4.120%
18	10.163	1369	1373	1380	rVB3	52523	77356	2.54%	0.249%
19	10.316	1396	1399	1404	rBV3	33284	37589	1.23%	0.121%
20	10.492	1424	1429	1433	rBV	144701	128278	4.21%	0.413%
21	10.716	1462	1467	1469	rBV2	56757	61184	2.01%	0.197%
22	10.875	1489	1494	1497	rBV	1987444	1914700	62.86%	6.162%
23	10.969	1507	1510	1520	rVB	181013	251808	8.27%	0.810%
24	11.422	1583	1587	1589	rBV	130123	118500	3.89%	0.381%
25	11.451	1589	1592	1594	rVB2	42802	43305	1.42%	0.139%
26	11.575	1609	1613	1616	rBV	1580382	1350708	44.35%	4.347%
27	11.598	1616	1617	1621	rVB	228785	135543	4.45%	0.436%
28	11.651	1621	1626	1628	rBV	47093	49653	1.63%	0.160%
29	11.845	1657	1659	1662	rVB	132678	90578	2.97%	0.291%
30	12.080	1695	1699	1701	rBV2	219094	201695	6.62%	0.649%
31	12.104	1701	1703	1708	rVB2	91384	83243	2.73%	0.268%
32	12.192	1714	1718	1720	rBV2	90629	110708	3.63%	0.356%
33	12.210	1720	1721	1725	rVB	49218	38623	1.27%	0.124%
34	12.251	1725	1728	1731	rBV	97725	91081	2.99%	0.293%
35	12.627	1788	1792	1793	rBV	91900	88154	2.89%	0.284%
36	12.716	1804	1807	1811	rBV3	60697	73755	2.42%	0.237%

LSC Area Percent Report

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Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPI

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-BF051424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.792	1816	1820	1824	rBV	801975	633340	20.79%	2.038%
38	12.863	1828	1832	1834	rBV3	31463	39874	1.31%	0.128%
39	12.969	1848	1850	1853	rVB2	40512	35421	1.16%	0.114%
40	13.022	1853	1859	1865	rBV	714671	823072	27.02%	2.649%
41	13.069	1865	1867	1871	rVB2	52649	60031	1.97%	0.193%
42	13.163	1875	1883	1886	rBV	3244643	2831804	92.98%	9.113%
43	13.233	1891	1895	1903	rBV5	69214	119061	3.91%	0.383%
44	13.327	1907	1911	1912	rBV3	56946	67422	2.21%	0.217%
45	13.351	1912	1915	1917	rVB2	85211	90600	2.97%	0.292%
46	13.416	1924	1926	1928	rBV	58998	42881	1.41%	0.138%
47	13.457	1928	1933	1935	rBV2	91540	97272	3.19%	0.313%
48	13.551	1946	1949	1951	rBV	73034	64357	2.11%	0.207%
49	13.580	1951	1954	1957	rVB	64276	56040	1.84%	0.180%
50	13.633	1957	1963	1966	rBV	248721	259756	8.53%	0.836%
51	13.716	1972	1977	1980	rBV3	46261	61139	2.01%	0.197%
52	13.857	1998	2001	2005	rVB	58563	66694	2.19%	0.215%
53	13.974	2015	2021	2023	rBV3	63661	92029	3.02%	0.296%
54	14.027	2028	2030	2031	rBV	40819	36268	1.19%	0.117%
55	14.222	2058	2063	2066	rBV2	1011833	1237792	40.64%	3.983%
56	14.251	2066	2068	2074	rVB	365423	309469	10.16%	0.996%
57	14.333	2079	2082	2085	rBV	53289	45722	1.50%	0.147%
58	14.439	2098	2100	2104	rBV2	32863	46092	1.51%	0.148%
59	14.610	2124	2129	2132	rBV	100064	109948	3.61%	0.354%
60	14.645	2132	2135	2137	rVB	64760	53309	1.75%	0.172%
61	14.680	2137	2141	2144	rBV3	25751	47182	1.55%	0.152%
62	14.745	2148	2152	2153	rVV2	59659	59634	1.96%	0.192%
63	14.763	2153	2155	2159	rVB2	48238	49644	1.63%	0.160%
64	15.316	2244	2249	2252	rBV	388482	611442	20.08%	1.968%
65	15.433	2265	2269	2274	rBV	87600	102067	3.35%	0.328%
66	15.645	2301	2305	2312	rVB	248286	333399	10.95%	1.073%
67	15.716	2312	2317	2323	rBV	356371	451178	14.81%	1.452%
68	15.786	2324	2329	2333	rVV	712302	970344	31.86%	3.123%
69	15.821	2333	2335	2341	rVB2	115484	143667	4.72%	0.462%
70	16.021	2365	2369	2378	rVB6	28124	59975	1.97%	0.193%
71	16.263	2405	2410	2414	rBV4	26620	47852	1.57%	0.154%
72	16.404	2430	2434	2440	rVB2	22739	38681	1.27%	0.124%
73	17.398	2597	2603	2612	rVB2	168208	367238	12.06%	1.182%
74	17.492	2615	2619	2627	rVB4	21477	47953	1.57%	0.154%
75	17.598	2632	2637	2644	rBV2	33595	65391	2.15%	0.210%
76	17.668	2644	2649	2654	rBV3	29598	58580	1.92%	0.189%

LSC Area Percent Report

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Misc :
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Instrument :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	17.792	2664	2670	2678	rVB6	42592	98786	3.24%	0.318%
78	17.898	2680	2688	2699	rVV	130264	293188	9.63%	0.944%
79	18.157	2726	2732	2736	rBV2	26947	50879	1.67%	0.164%

Sum of corrected areas: 31073650

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052024\
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Misc :
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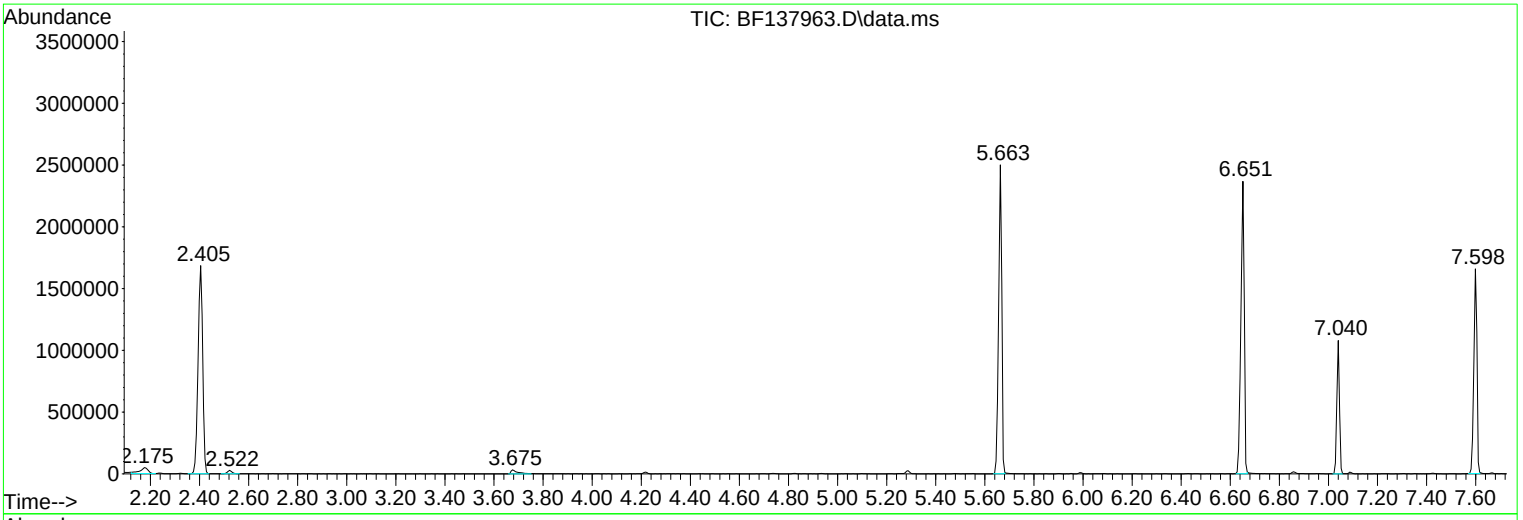
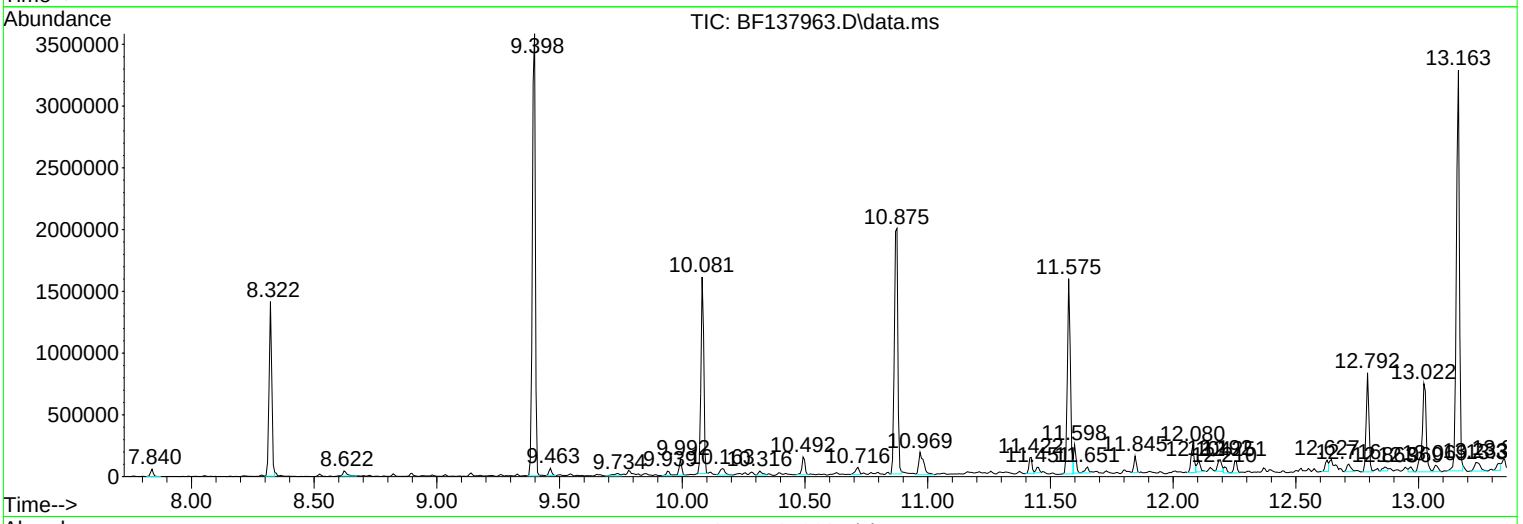
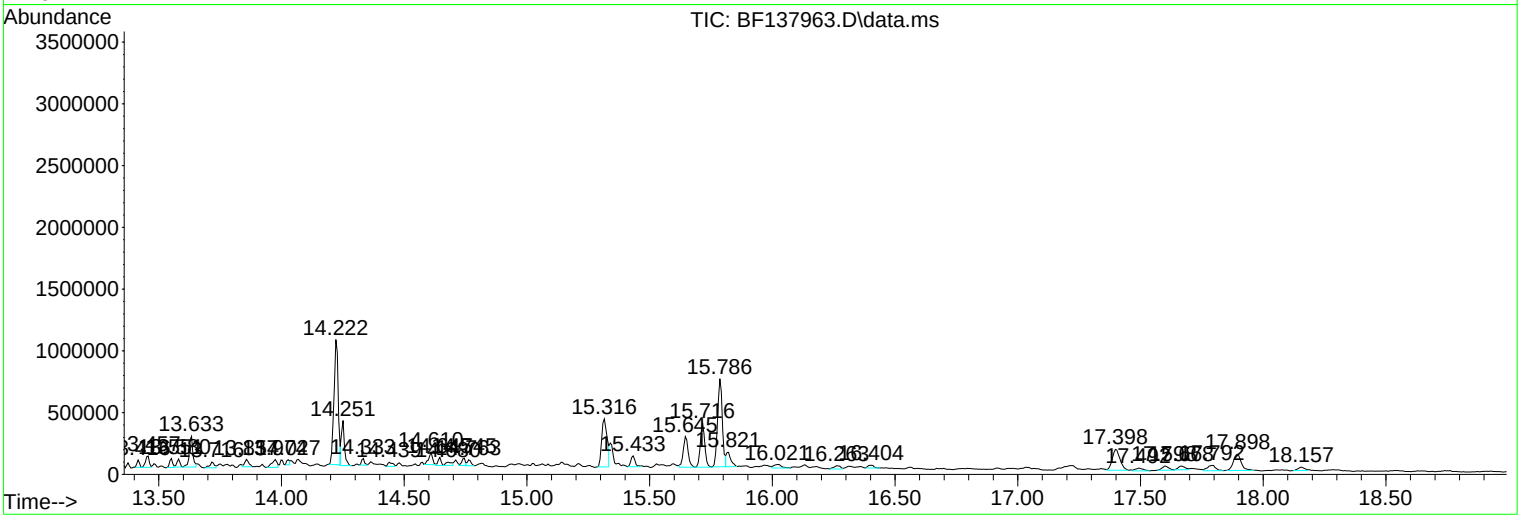
Instrument :
BNA_F
ClientSampleId :
WCS-TPI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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\BF052024\
Data File : BF137963.D
Acq On : 20 May 2024 17:08
Operator : CG\JU
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

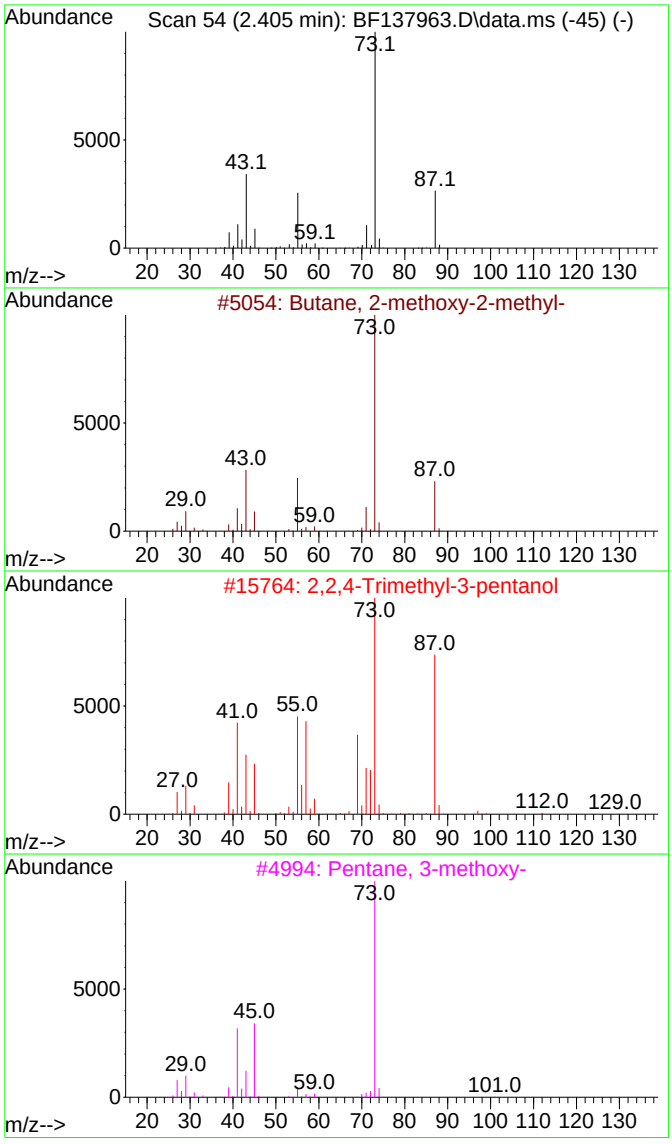
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

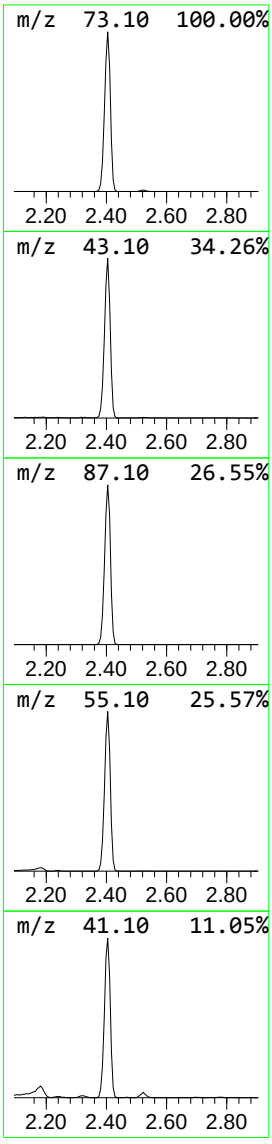
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.405	54.67 ng	2212120	1,4-Dichlorobenzene-d4	7.040

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

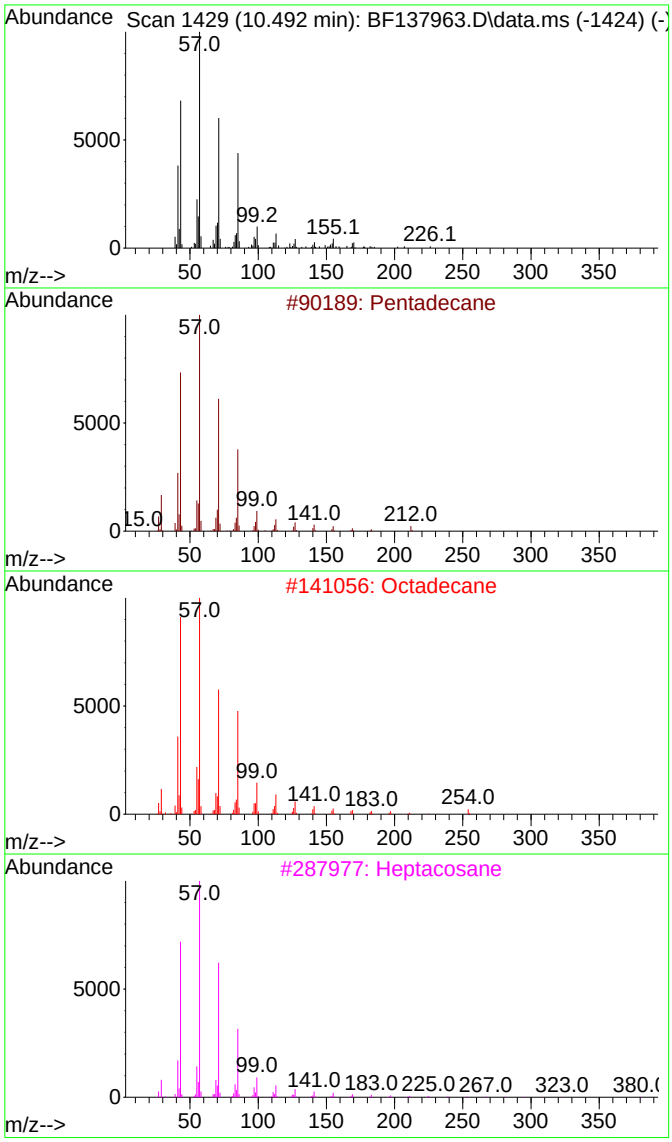
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

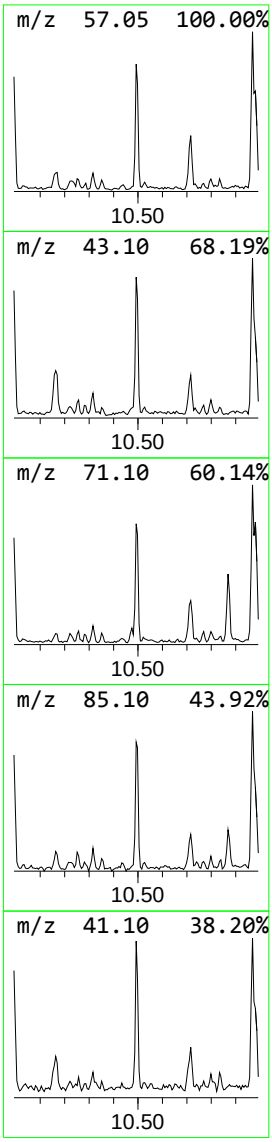
****

Peak Number 3 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.492	2.00 ng	128278	Acenaphthene-d10	10.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Dodecane	170	C12H26	000112-40-3	90





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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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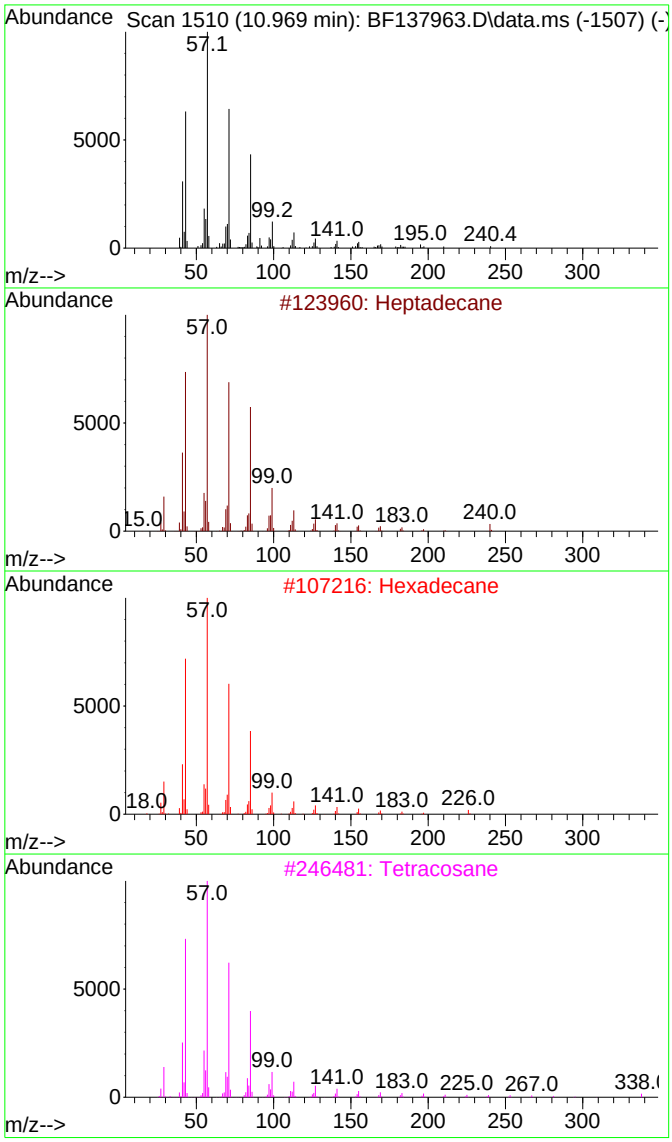
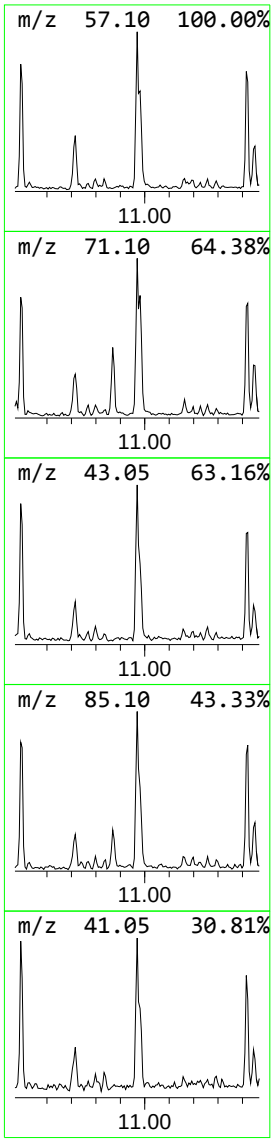
Peak Number 4 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.969	3.73 ng	251808	Phenanthrene-d10	11.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	97
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Tetradecane	198	C14H30	000629-59-4	91
5	Octadecane	254	C18H38	000593-45-3	91





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

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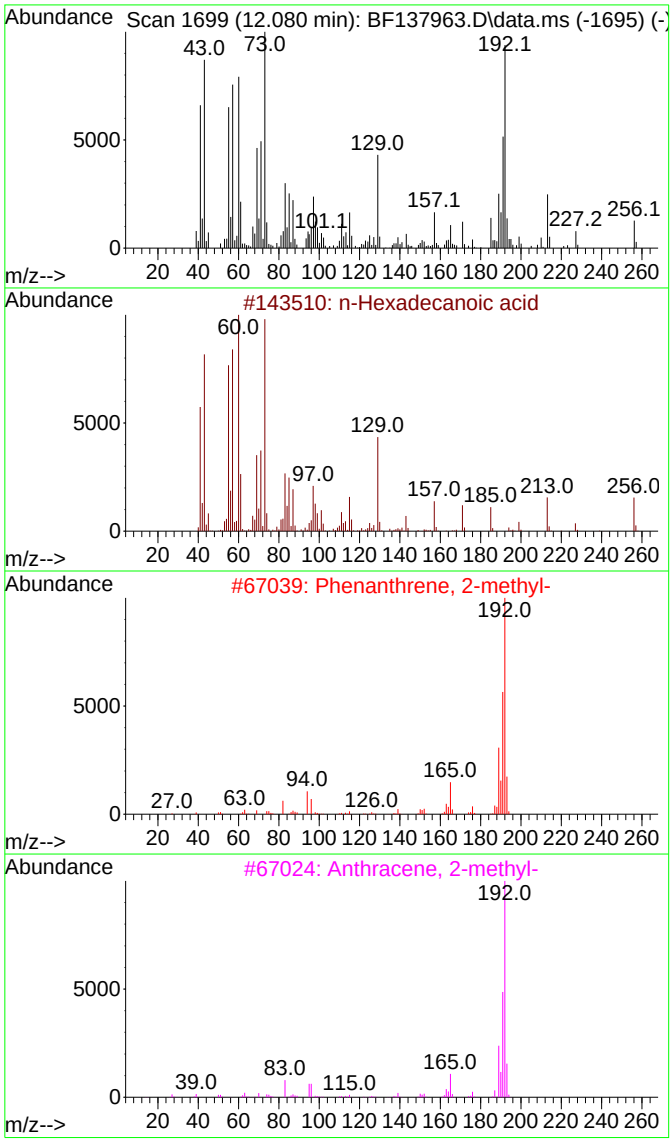
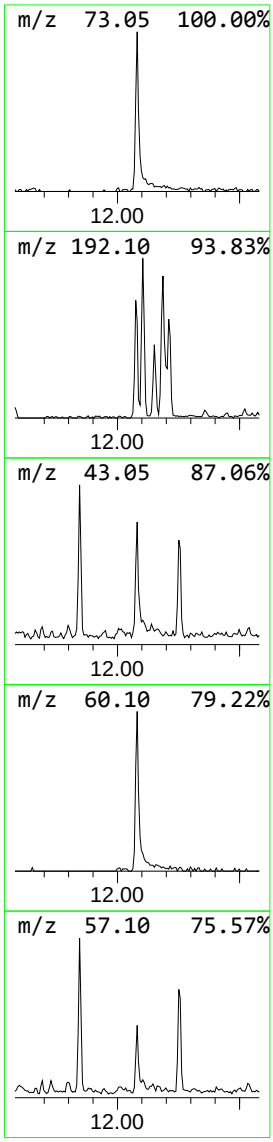
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.081	2.99 ng	201695	Phenanthrene-d10	11.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	62
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	62





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

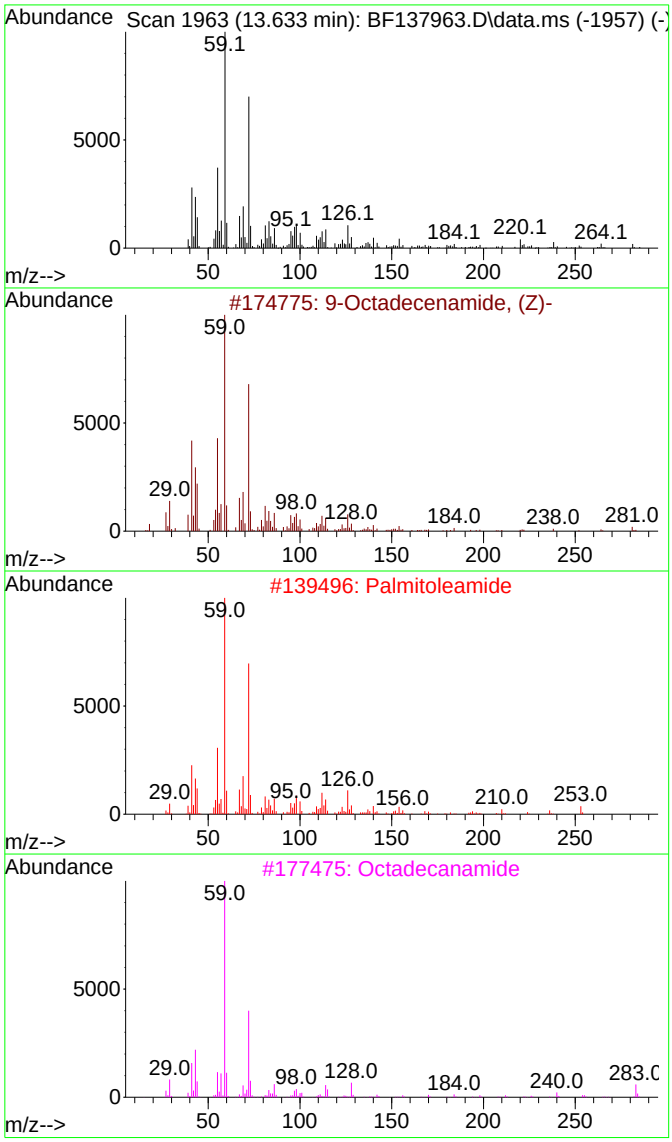
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

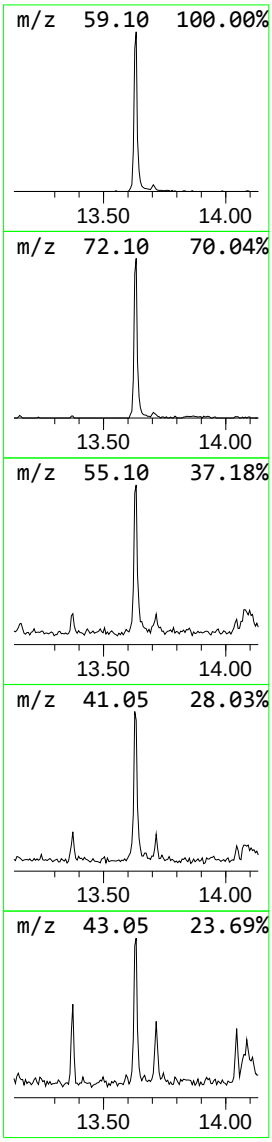
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.633	4.20 ng	259756	Chrysene-d12	14.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Palmitoleamide	253	C16H31NO	106010-22-4	78
3	Octadecanamide	283	C18H37NO	000124-26-5	72
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5	9-Octadecenamide	281	C18H35NO	003322-62-1	59





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Data File : BF137963.D
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Operator : CG\JU
Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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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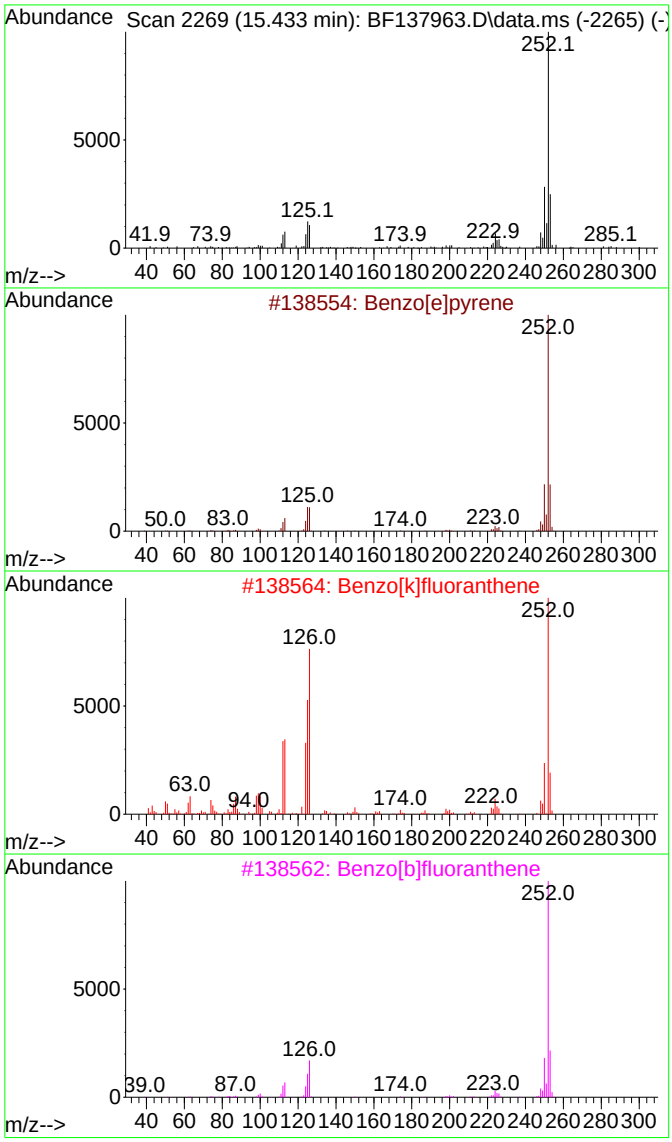
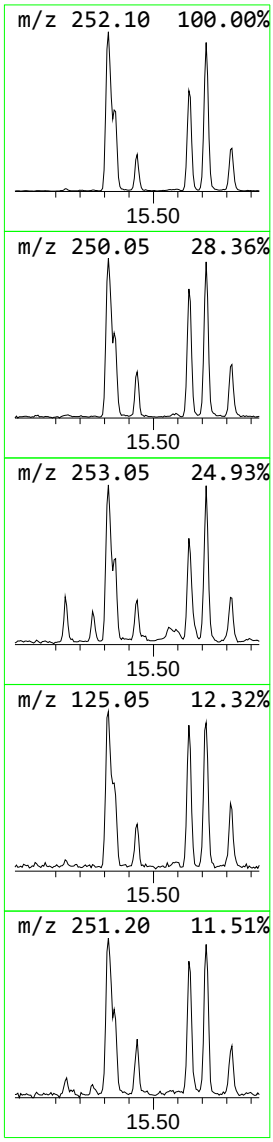
Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	2.10 ng	102067	Perylene-d12	15.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





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Acq On : 20 May 2024 17:08
Operator : CG\JU
Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

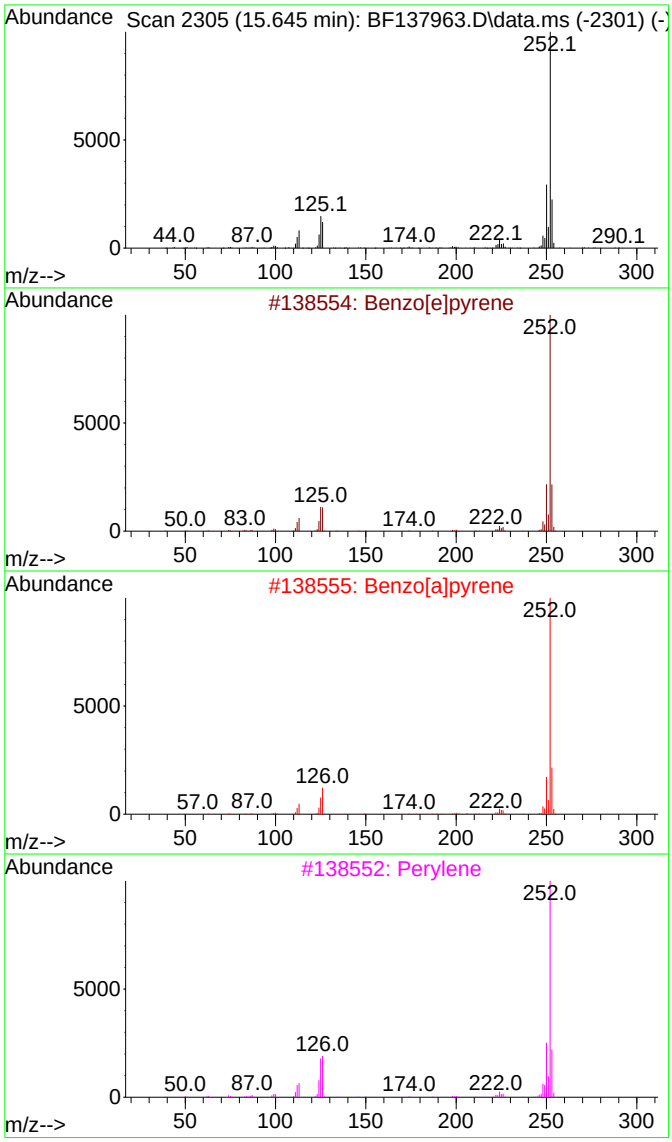
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

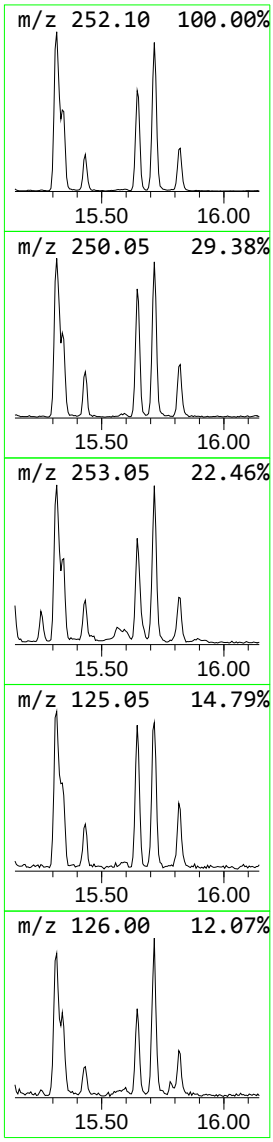
****

Peak Number 8 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	6.87 ng	333399	Perylene-d12	15.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052024\
Data File : BF137963.D
Acq On : 20 May 2024 17:08
Operator : CG\JU
Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

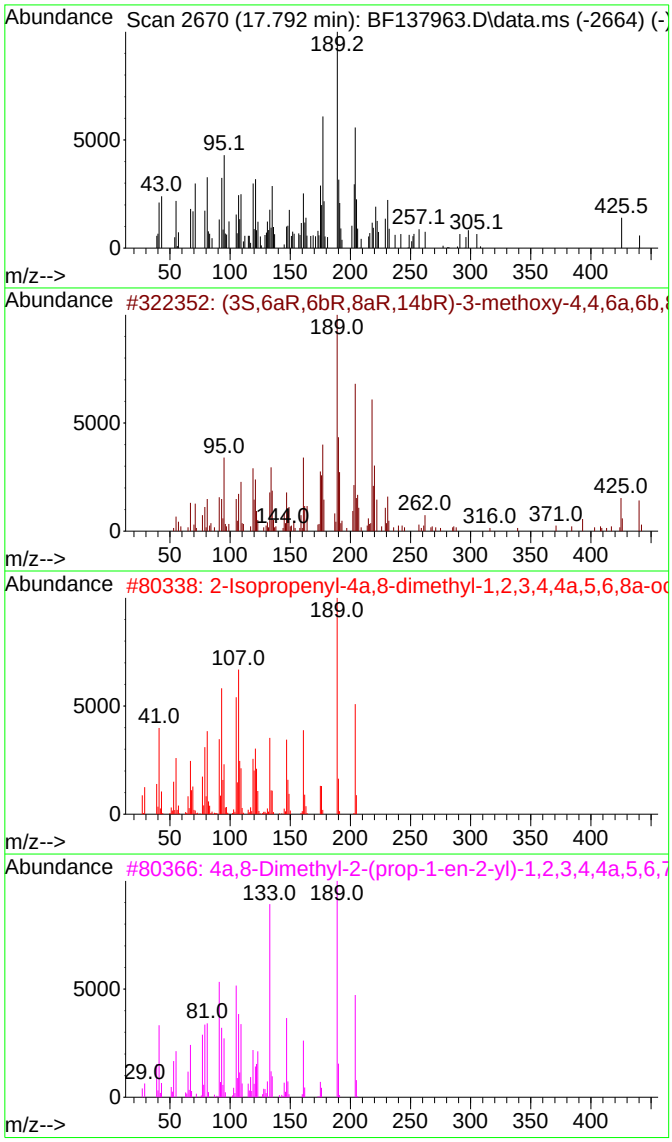
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

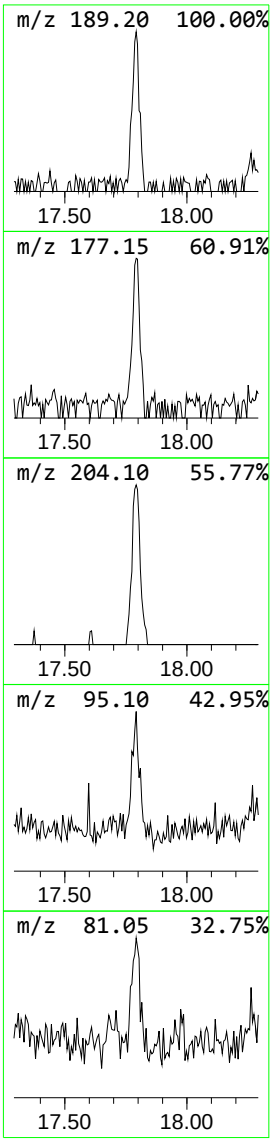
****

Peak Number 9 (3S,6aR,6bR,8aR,14bR)-3-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.792	2.04 ng	98786	Perylene-d12	15.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,6aR,6bR,8aR,14bR)-3-methoxy-...	440	C31H52O	1000441-97-8	55
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	46
3	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	45
4	3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	38
5	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052024\
Data File : BF137963.D
Acq On : 20 May 2024 17:08
Operator : CG\JU
Sample : P2512-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.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...	2.405	54.7	ng	2212120	1	7.040	809264	20.0
Pentadecane	10.492	2.0	ng	128278	3	10.081	1280320	20.0
Heptadecane	10.969	3.7	ng	251808	4	11.575	1350710	20.0
n-Hexadecanoic ...	12.081	3.0	ng	201695	4	11.575	1350710	20.0
9-Octadecenamid...	13.633	4.2	ng	259756	5	14.227	1237790	20.0
Benzo[e]pyrene	15.433	2.1	ng	102067	6	15.786	970344	20.0
Perylene	15.645	6.9	ng	333399	6	15.786	970344	20.0
(3S,6aR,6bR,8aR...	17.792	2.0	ng	98786	6	15.786	970344	20.0