LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-HRH-COMP-02

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-BF052025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142508.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	488	496	508	rBV	127828	181844	11.09%	1.180%
2	5.510	558	564	569	rBV	975190	1249964	76.22%	8.112%
3	6.516	729	735	746	rBV	1088326	1456524	88.81%	9.453%
4	6.898	794	800	805	rBV	504517	637211	38.85%	4.135%
5	7.457	888	895	900	rBV	802140	1049116	63.97%	6.809%
6	7.710	934	938	946	rBV	20789	27524	1.68%	0.179%
7	8.181	1012	1018	1023	rBV	654100	838879	51.15%	5.444%
8	8.392	1050	1054	1062	rBV2	13484	18655	1.14%	0.121%
9	9.251	1195	1200	1205	rBV	1313550	1640042	100.00%	10.644%
10	9.439	1229	1232	1238	rVB	14687	18207	1.11%	0.118%
11	9.569	1250	1254	1263	rBV2	207621	356837	21.76%	2.316%
12	9.639	1263	1266	1270	rVV2	11745	16743	1.02%	0.109%
13	9.692	1270	1275	1280	rVB	22133	26951	1.64%	0.175%
14	9.875	1303	1306	1310	rVB3	14990	17937	1.09%	0.116%
15	9.933	1310	1316	1321	rBV	749471	937850	57.18%	6.086%
16	10.610	1426	1431	1434	rBV	220477	269064	16.41%	1.746%
17	10.645	1434	1437	1441	rVB	147012	169888	10.36%	1.103%
18	10.722	1444	1450	1455	rVB	757039	946216	57.69%	6.141%
19	11.421	1564	1569	1577	rVV	687539	932294	56.85%	6.050%
20	11.498	1577	1582	1600	rVB5	14751	46055	2.81%	0.299%
21	11.945	1648	1658	1670	rVV	232186	442397	26.97%	2.871%
22	12.033	1670	1673	1682	rVB2	13552	26469	1.61%	0.172%
23	12.521	1750	1756	1760	rVB2	27636	37476	2.29%	0.243%
24	12.633	1770	1775	1780	rBV	84160	117175	7.14%	0.760%
25	12.727	1787	1791	1800	rBV	21421	37192	2.27%	0.241%
26	12.863	1805	1814	1819	rBV	66951	102155	6.23%	0.663%
27	12.968	1827	1832	1834	rBV	21002	27767	1.69%	0.180%
28	13.010	1834	1839	1844	rVB	941632	1223409	74.60%	7.940%
29	13.327	1889	1893	1900	rVB	53899	74988	4.57%	0.487%
30	13.439	1907	1912	1915	rBV	368765	484433	29.54%	3.144%
31	13.468	1915	1917	1927	rVV2	122746	199492	12.16%	1.295%
32	13.580	1931	1936	1946	rVB5	9989	19315	1.18%	0.125%
33	13.904	1987	1991	1994	rBV2	42354	60478	3.69%	0.392%
34	13.939	1994	1997	2002	rVB3	34245	48752	2.97%	0.316%
35	14.062	2011	2018	2032	rVB	484340	692421	42.22%	4.494%
36	14.221	2039	2045	2053	rBV4	11850	25696	1.57%	0.167%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-HRH-COMP-02

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-BF052025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.462	2081	2086	2088	rBV2	31750	44735	2.73%	0.290%
38	14.492	2088	2091	2094	rVV2	27026	34498	2.10%	0.224%
39	14.527	2094	2097	2102	rVB3	13810	19688	1.20%	0.128%
40	14.692	2121	2125	2129	rVB	14873	18936	1.15%	0.123%
41	14.839	2145	2150	2155	rVB3	13002	22630	1.38%	0.147%
42	14.992	2172	2176	2181	rBV2	17316	25880	1.58%	0.168%
43	15.115	2192	2197	2206	rBV	31957	74308	4.53%	0.482%
44	15.192	2206	2210	2212	rBV	17066	23493	1.43%	0.152%
45	15.421	2245	2249	2255	rBV	15755	25194	1.54%	0.164%
46	15.486	2256	2260	2265	rVV	23312	34980	2.13%	0.227%
47	15.557	2265	2272	2284	rVB	366071	600695	36.63%	3.898%
48	16.033	2349	2353	2358	rVB	16947	26332	1.61%	0.171%

Sum of corrected areas: 15408785

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Instrument :
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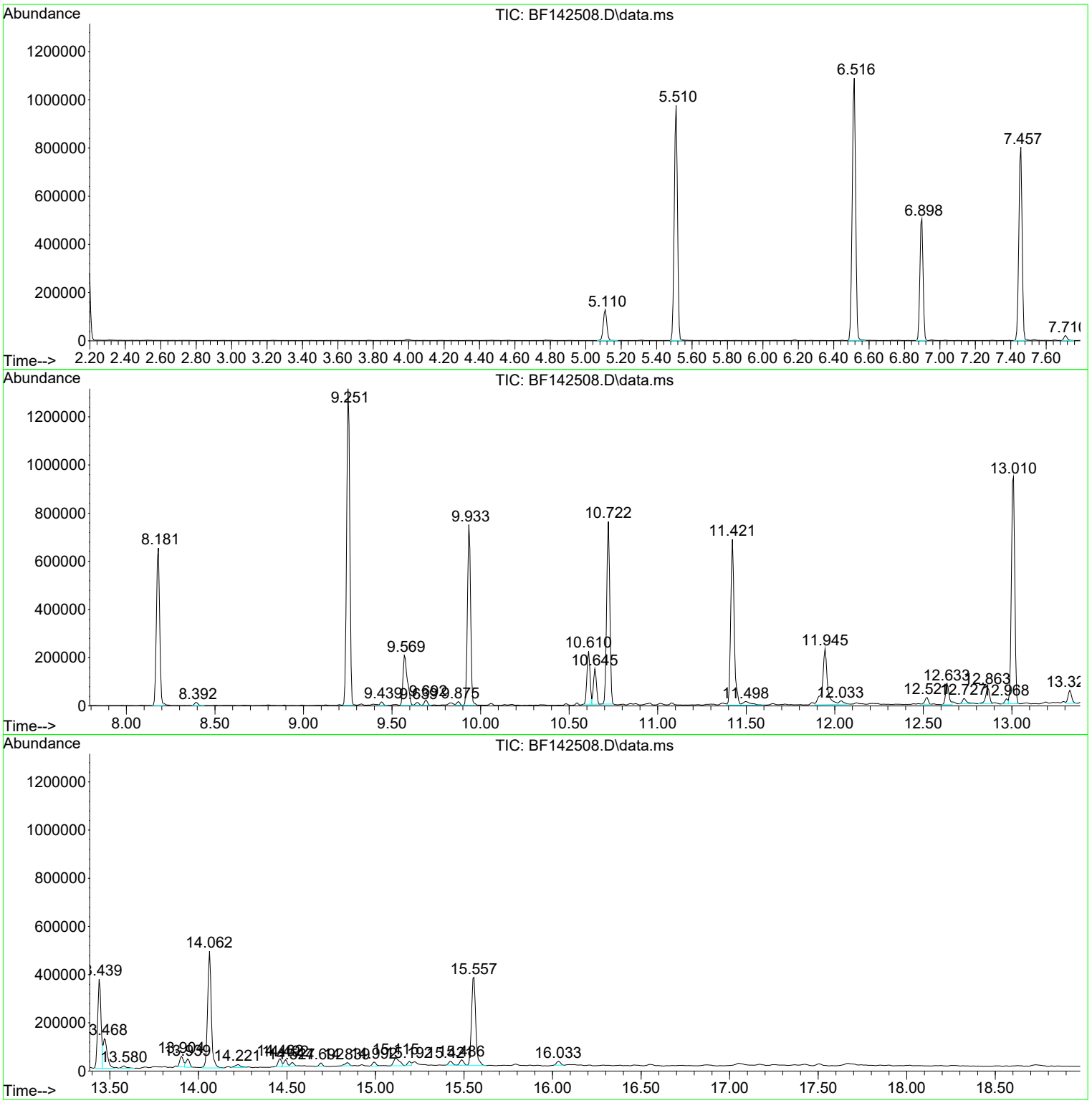
ClientSampleId :
PL-HRH-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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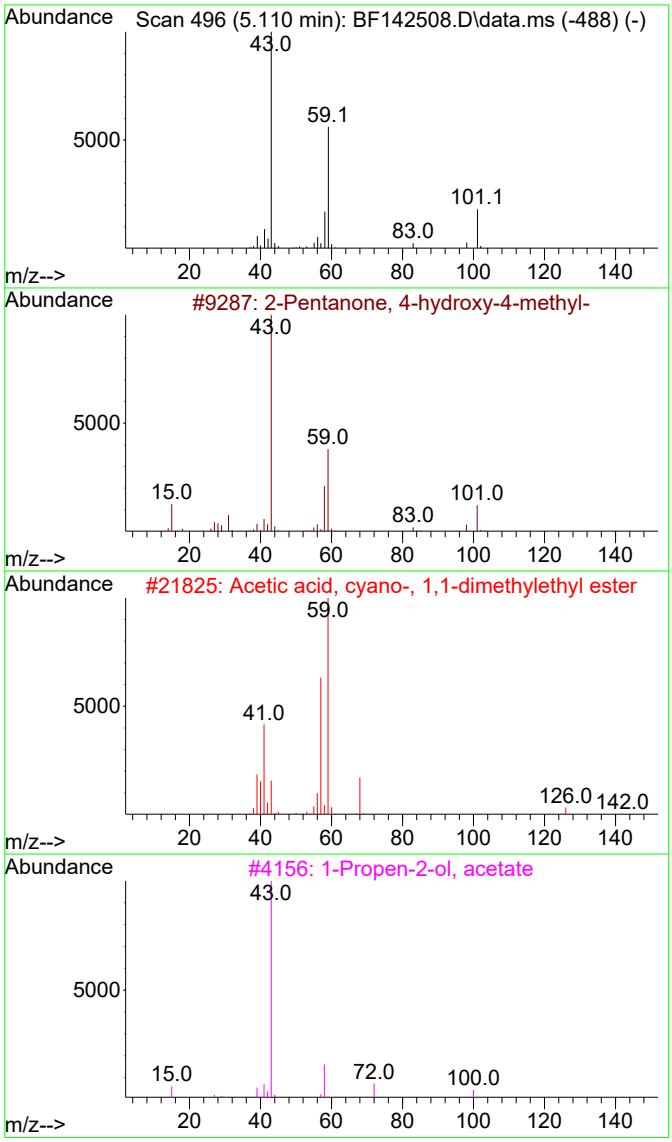
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

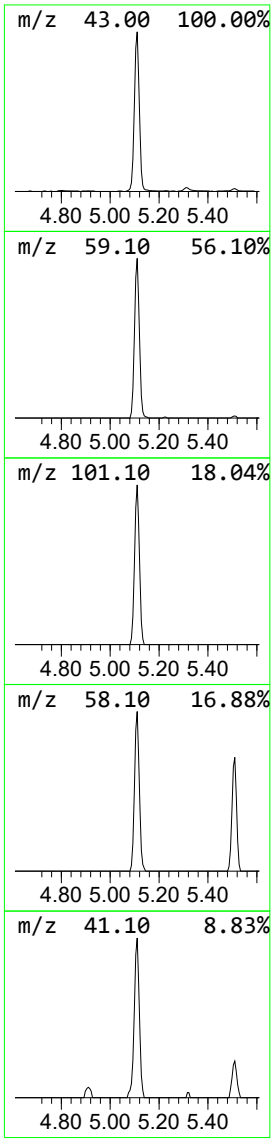
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.71 ng	181844	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
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Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-HRH-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

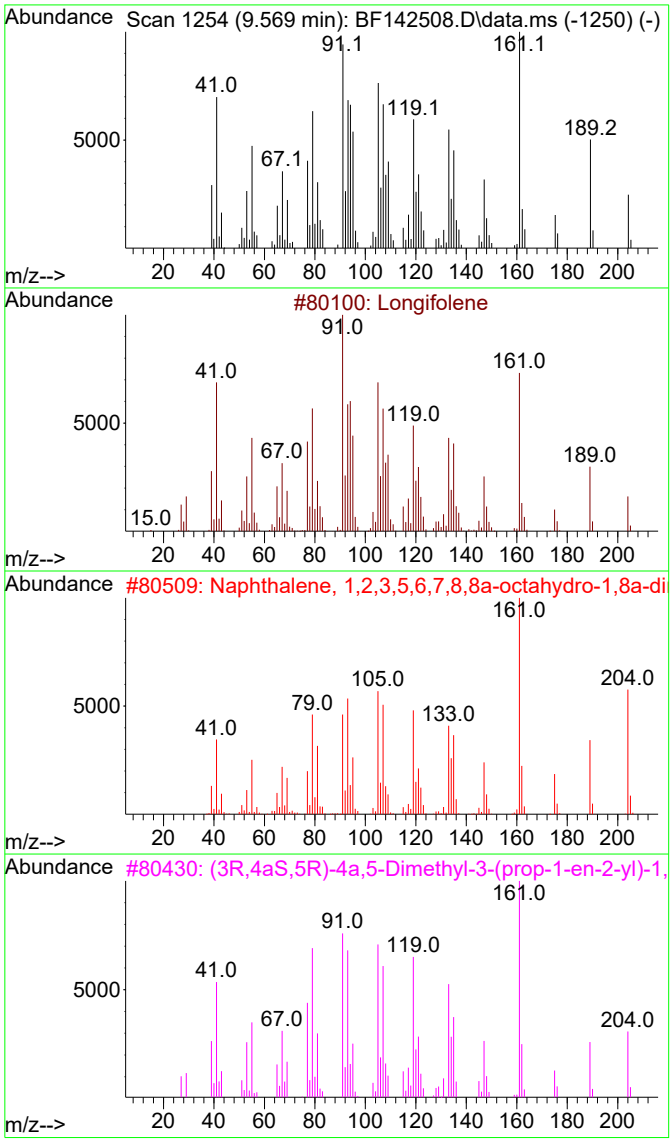
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

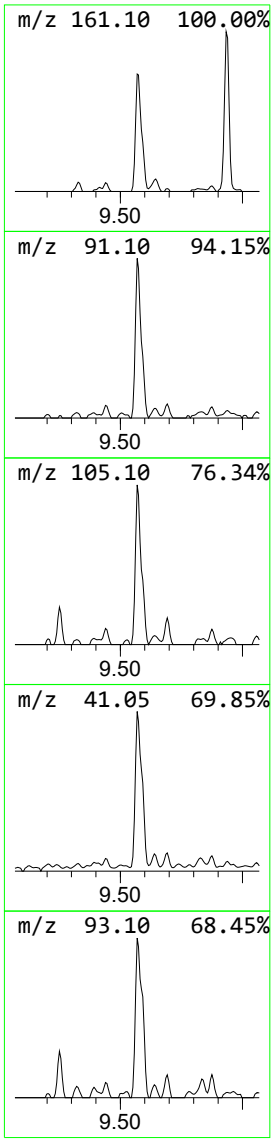
****

Peak Number 2 Longifolene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.569	7.61 ng	356837	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolene	204	C15H24	000475-20-7	99
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	96
3	(3R,4aS,5R)-4a,5-Dimethyl-3-(pro...	204	C15H24	024741-64-8	95
4	Aromandendrene	204	C15H24	000489-39-4	90
5	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-HRH-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

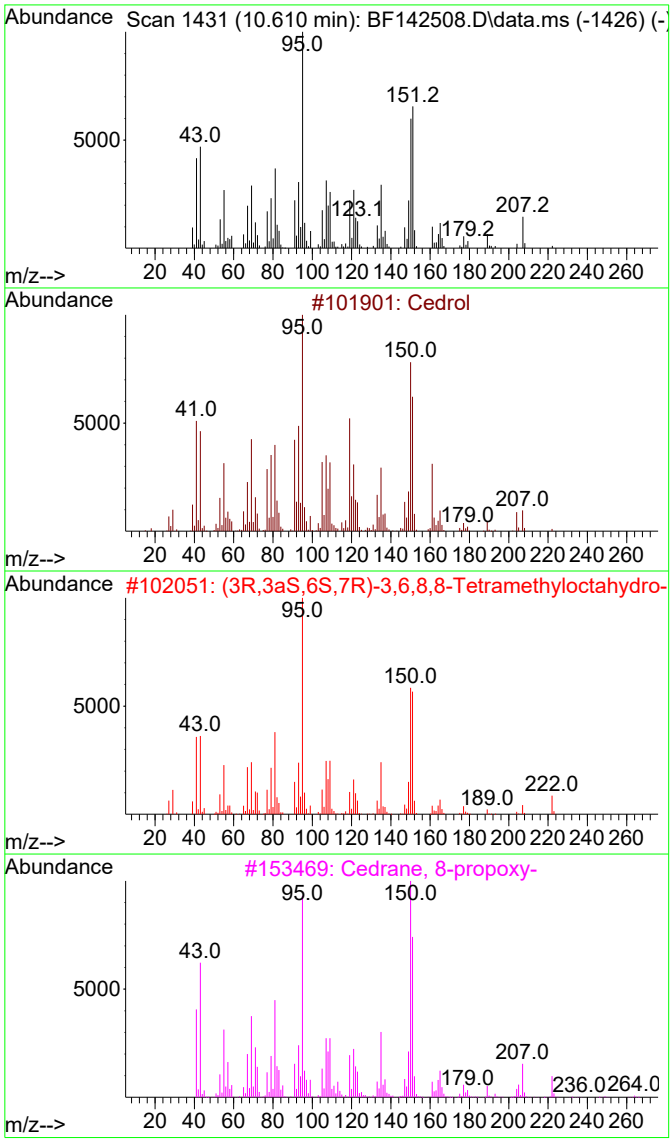
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

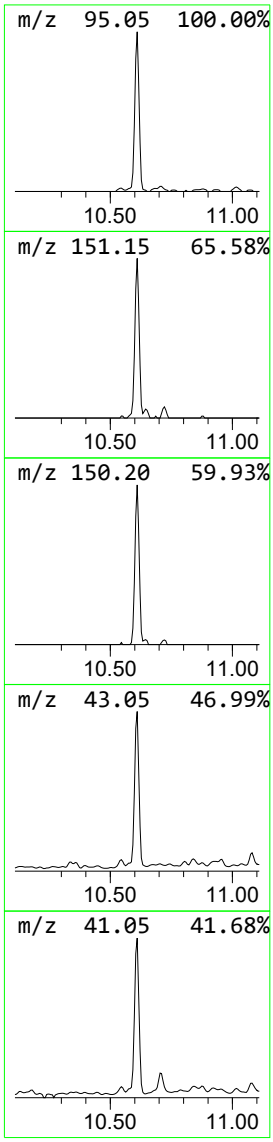
****

Peak Number 3 Cedrol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	5.74 ng	269064	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cedrol	222	C15H26O	000077-53-2	93
2	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	91
3	Cedrane, 8-propoxy-	264	C18H32O	019870-75-8	87
4	Piperonylamine	151	C8H9NO2	002620-50-0	38
5	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
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Acq On : 22 May 2025 14:09
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Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

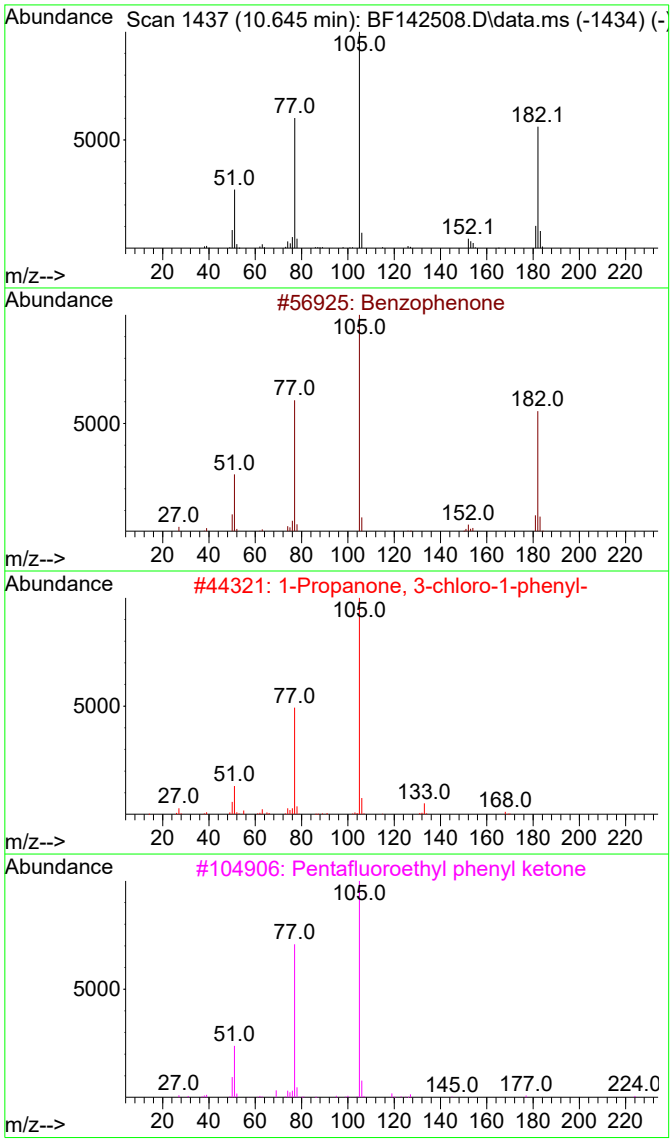
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

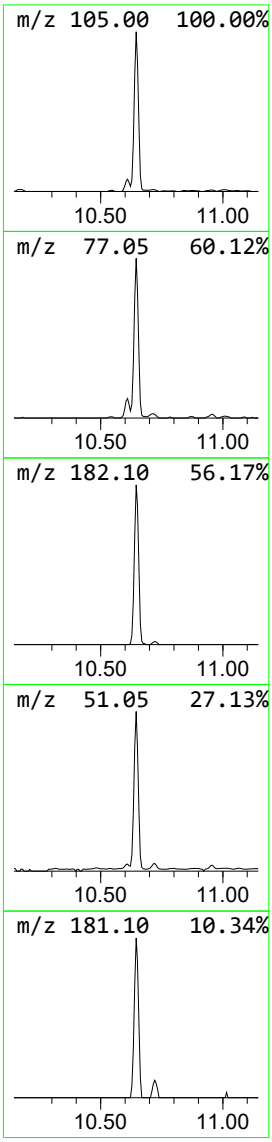
****

Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	3.62 ng	169888	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
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Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

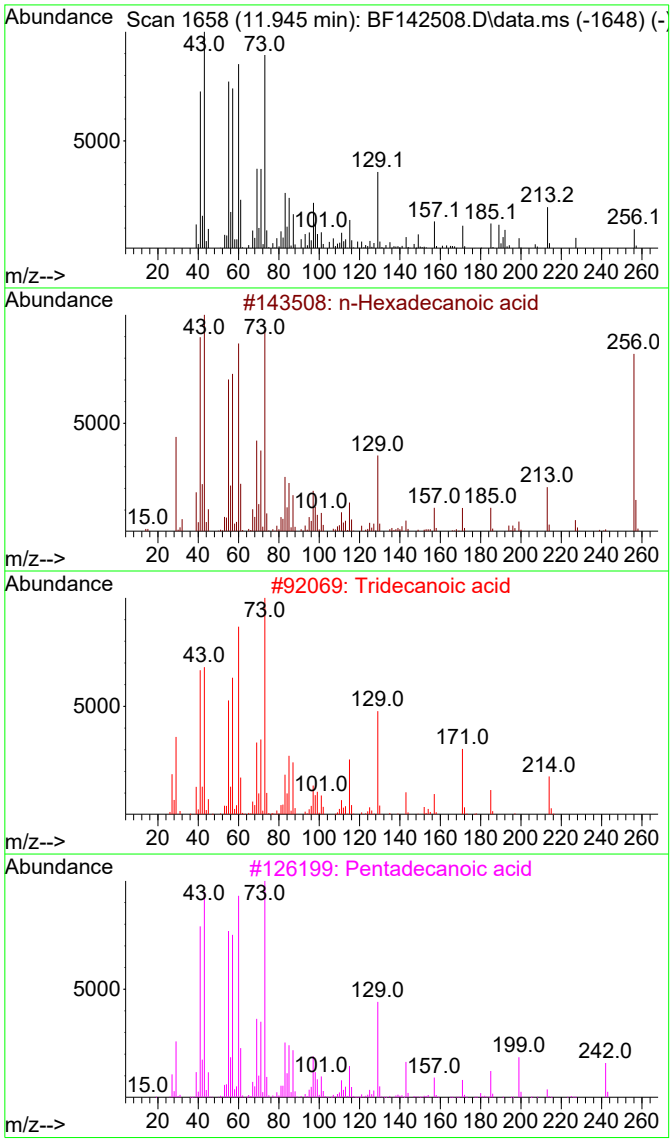
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

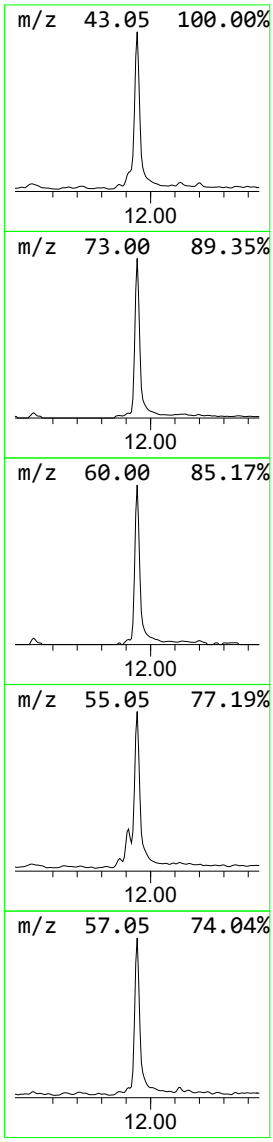
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	9.49 ng	442397	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





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Instrument :
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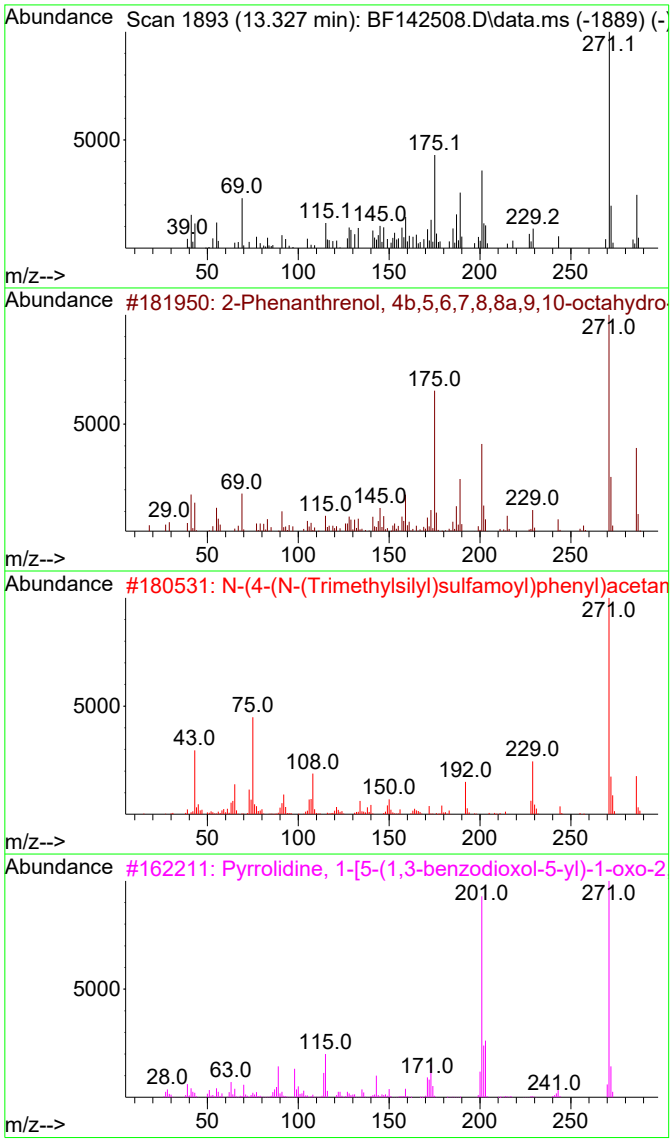
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

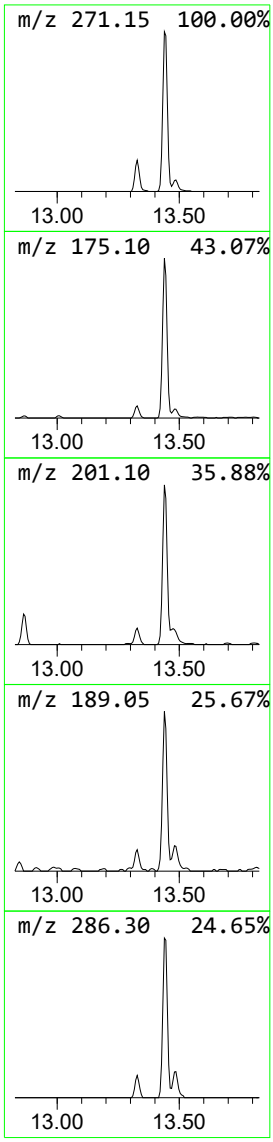
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	2.17 ng	74988	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	70
2	N-(4-(N-(Trimethylsilyl)sulfamoy...	286	C11H18N2O3SSi	1000473-84-9	43
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	43
4	Normorphine	271	C16H17NO3	000466-97-7	38
5	3-Phenyl-5-(tetramethyl-1,3,2-di...	271	C15H18BNO3	1000434-90-0	38





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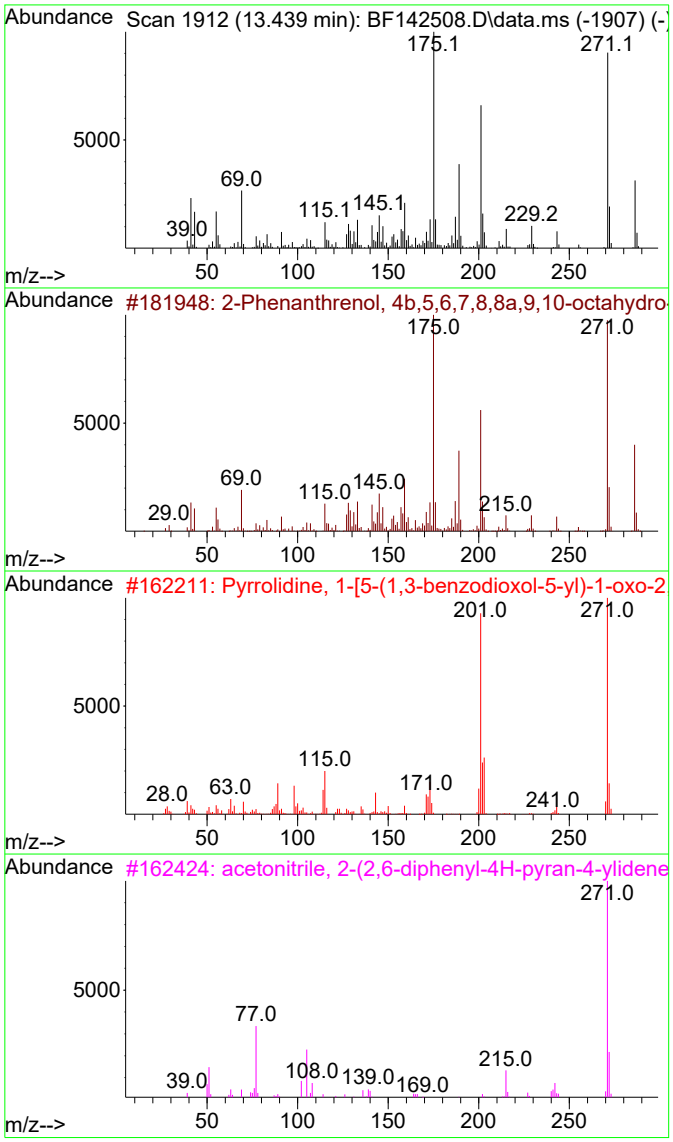
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

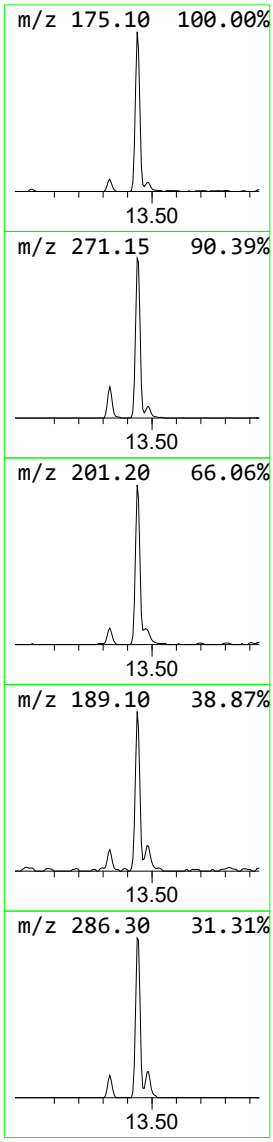
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown13.439 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	13.99 ng	484433	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	27
3	acetonitrile, 2-(2,6-diphenyl-4H...	271	C19H13NO	1010397-00-1	20
4	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	18
5	2-(1-Hydroxynaphthyl-2)quinoline	271	C19H13NO	024641-28-9	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

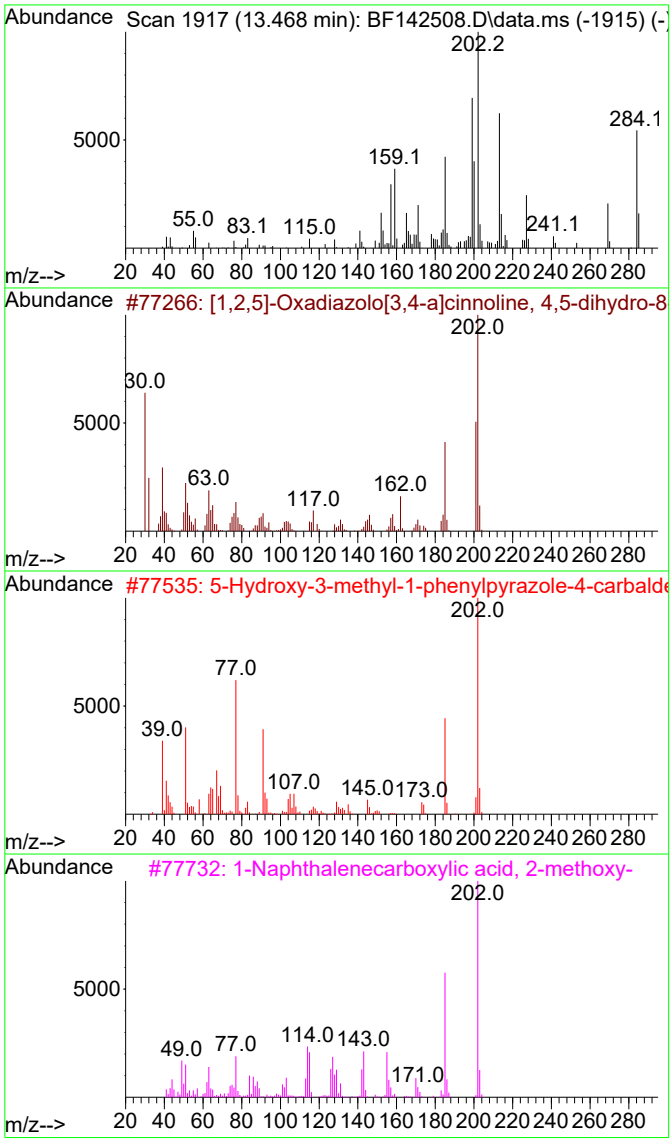
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

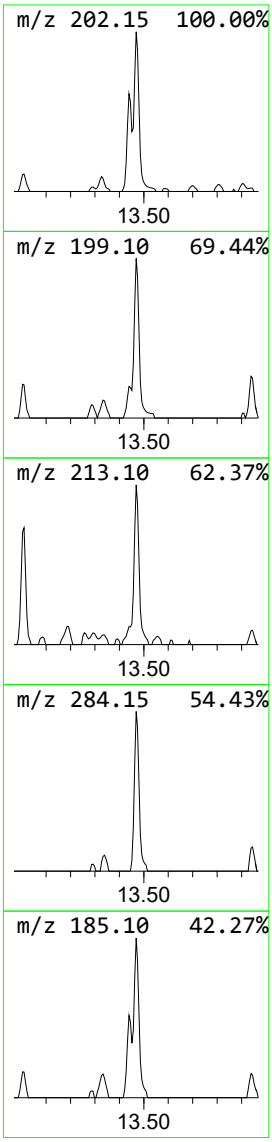
****

Peak Number 9 unknown13.468 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.468	5.76 ng	199492	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	38
2	5-Hydroxy-3-methyl-1-phenylpyraz...	202	C11H10N2O2	060484-29-9	22
3	1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	22
4	Desmetryn	213	C8H15N5S	001014-69-3	15
5	1-Chloro-2-di-tert-butyl-silylox...	270	C14H23ClOSi	1010292-69-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-HRH-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

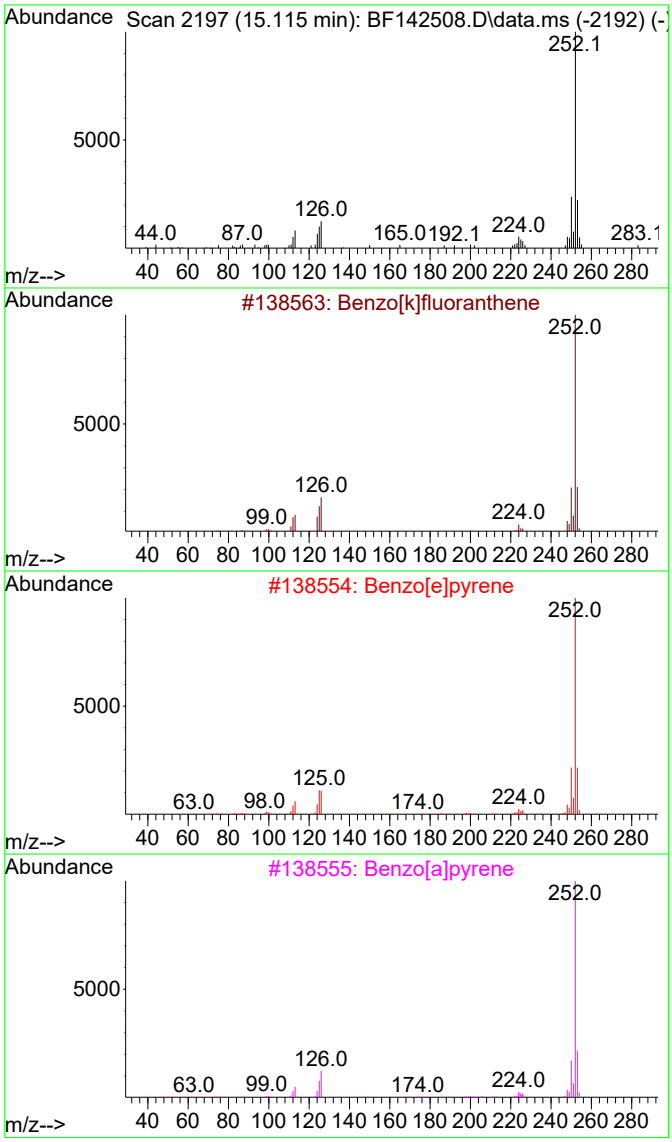
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

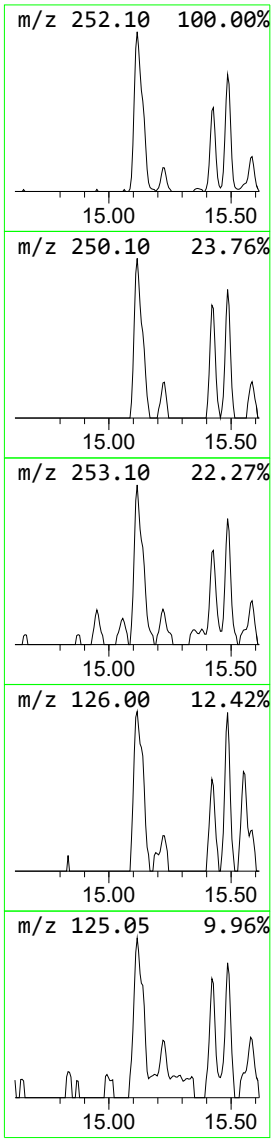
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	2.47 ng	74308	Perylene-d12	15.557

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052225\
Data File : BF142508.D
Acq On : 22 May 2025 14:09
Operator : RC/JU
Sample : Q2080-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-HRH-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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-...	5.110	5.7	ng	181844	1	6.898	637211	20.0
Longifolene	9.569	7.6	ng	356837	3	9.933	937850	20.0
Cedrol	10.610	5.7	ng	269064	3	9.933	937850	20.0
Benzophenone	10.645	3.6	ng	169888	3	9.933	937850	20.0
n-Hexadecanoic ...	11.945	9.5	ng	442397	4	11.422	932294	20.0
2-Phenanthrenol...	13.327	2.2	ng	74988	5	14.063	692421	20.0
unknown13.439	13.439	14.0	ng	484433	5	14.063	692421	20.0
unknown13.468	13.468	5.8	ng	199492	5	14.063	692421	20.0
Benzo[e]pyrene	15.115	2.5	ng	74308	6	15.557	600695	20.0