LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135635.D
Acq On : 06 Oct 2023 18:25
Operator : CG\JU
Sample : 04736-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11991

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.787	115	119	127	rBV	25618	44727	1.18%	0.129%
2	4.340	379	383	403	rBV	150694	233193	6.16%	0.670%
3	4.975	484	491	510	rBV	2298512	3765870	99.56%	10.820%
4	5.381	556	560	578	rBV	3437382	3654779	96.62%	10.501%
5	5.763	621	625	632	rBV	108319	107487	2.84%	0.309%
6	6.392	728	732	758	rBV	3515990	3782600	100.00%	10.868%
7	6.598	764	767	783	rBV2	17122	47400	1.25%	0.136%
8	6.739	787	791	801	rVB	1086396	951090	25.14%	2.733%
9	7.304	883	887	899	rBV	2308023	2454684	64.89%	7.053%
10	8.016	1004	1008	1017	rBV	1431814	1285062	33.97%	3.692%
11	9.098	1187	1192	1195	rBV	4040990	3711659	98.12%	10.664%
12	9.216	1208	1212	1222	rVB	200348	201844	5.34%	0.580%
13	9.775	1303	1307	1310	rBV	1605996	1371844	36.27%	3.942%
14	10.569	1438	1442	1458	rBV	2269161	2343499	61.95%	6.733%
15	11.269	1557	1561	1563	rBV	1618048	1368877	36.19%	3.933%
16	11.292	1563	1565	1569	rVV	219463	184160	4.87%	0.529%
17	11.345	1570	1574	1578	rVB	59542	61398	1.62%	0.176%
18	11.804	1649	1652	1658	rBV	354482	368360	9.74%	1.058%
19	11.886	1663	1666	1668	rBV	46815	41950	1.11%	0.121%
20	12.374	1743	1749	1753	rBV5	70113	103413	2.73%	0.297%
21	12.486	1765	1768	1773	rBV	405044	398763	10.54%	1.146%
22	12.592	1784	1786	1792	rBV3	50637	78842	2.08%	0.227%
23	12.721	1802	1808	1813	rVB	393979	430519	11.38%	1.237%
24	12.863	1826	1832	1836	rBV	3113891	3037990	80.31%	8.729%
25	12.939	1841	1845	1850	rBV2	40390	59067	1.56%	0.170%
26	13.051	1857	1864	1868	rBV2	93257	144699	3.83%	0.416%
27	13.121	1873	1876	1878	rVV	68998	62614	1.66%	0.180%
28	13.157	1878	1882	1889	rVB3	64696	89581	2.37%	0.257%
29	13.251	1895	1898	1900	rBV	43258	38866	1.03%	0.112%
30	13.574	1950	1953	1958	rVB	46255	52869	1.40%	0.152%
31	13.680	1968	1971	1973	rBV	52661	50741	1.34%	0.146%
32	13.851	1994	2000	2006	rBV4	43082	114863	3.04%	0.330%
33	13.927	2006	2013	2016	rVV2	1021488	1192516	31.53%	3.426%
34	13.957	2016	2018	2026	rVB	291627	266946	7.06%	0.767%
35	14.398	2088	2093	2096	rBV6	41900	81253	2.15%	0.233%
36	14.498	2107	2110	2111	rBV	68398	60228	1.59%	0.173%

LSC Area Percent Report

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Operator : CG\JU
Sample : 04736-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.557	2116	2120	2124	rBV	307727	343142	9.07%	0.986%
38	14.651	2133	2136	2137	rBV2	59267	52876	1.40%	0.152%
39	14.680	2138	2141	2148	rVB	118097	227516	6.01%	0.654%
40	14.733	2148	2150	2153	rBV	60047	61821	1.63%	0.178%
41	14.821	2162	2165	2168	rVB2	44503	44004	1.16%	0.126%
42	14.974	2187	2191	2194	rBV	222815	331528	8.76%	0.953%
43	15.274	2238	2242	2248	rVB	133753	164946	4.36%	0.474%
44	15.339	2249	2253	2258	rBV	134794	166070	4.39%	0.477%
45	15.398	2258	2263	2268	rBV	669571	890208	23.53%	2.558%
46	15.839	2334	2338	2344	rBV2	39701	63402	1.68%	0.182%
47	16.892	2511	2517	2522	rBV2	54132	117960	3.12%	0.339%
48	17.339	2589	2593	2605	rVB	39127	96775	2.56%	0.278%

Sum of corrected areas: 34804501

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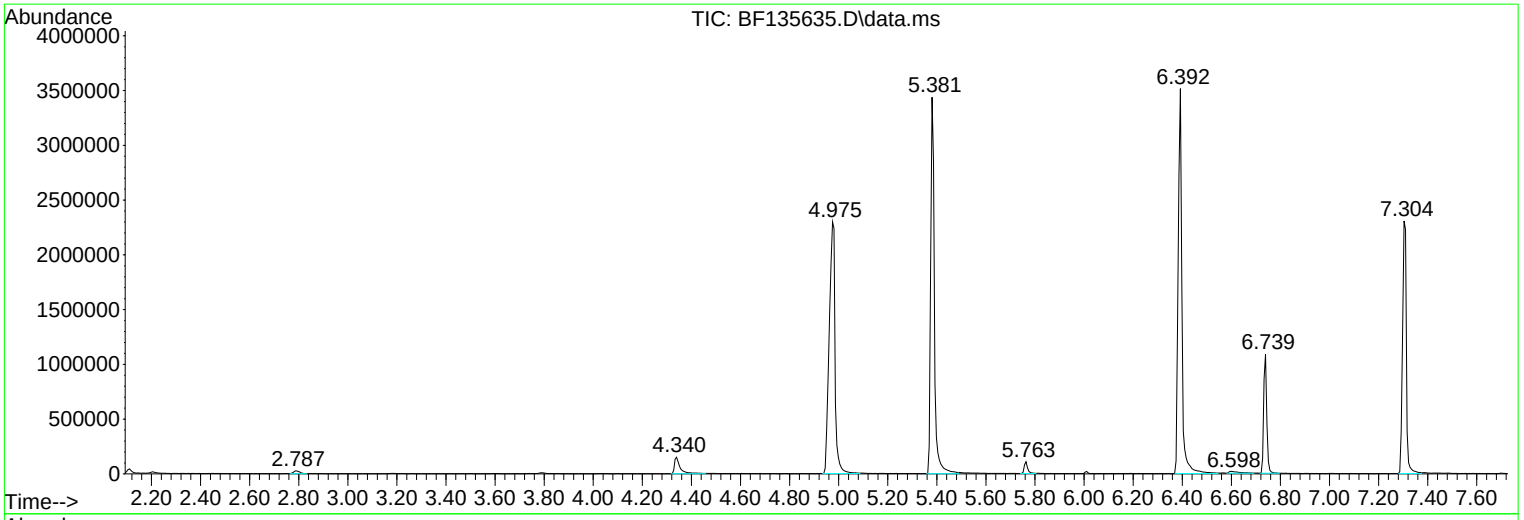
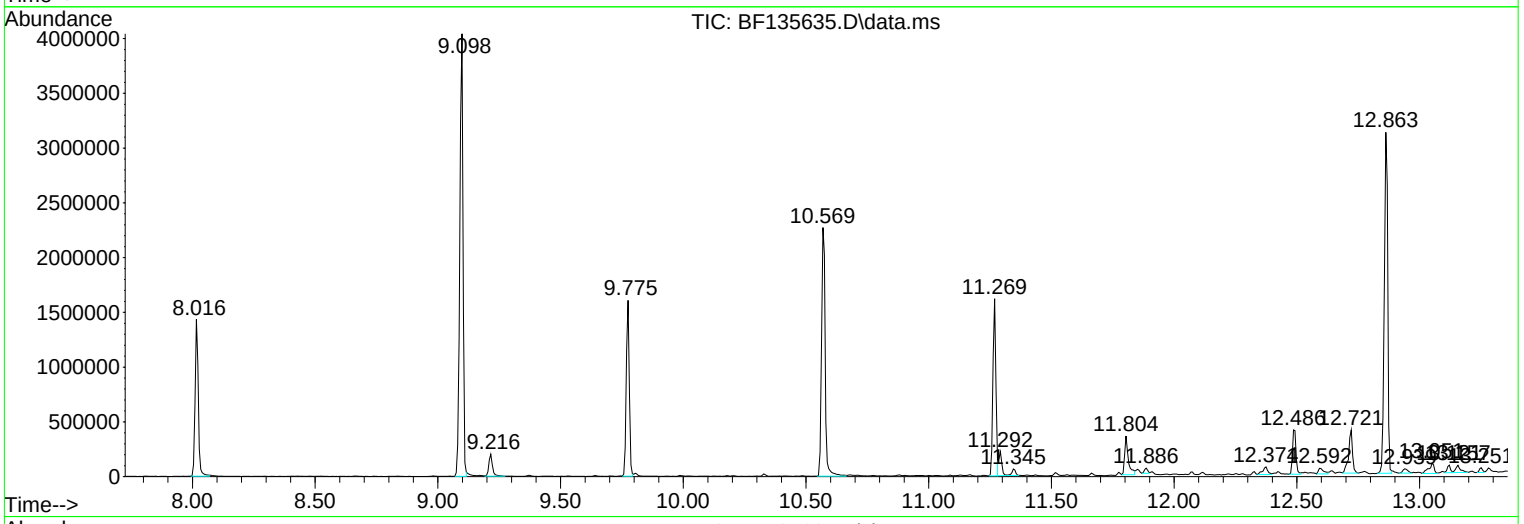
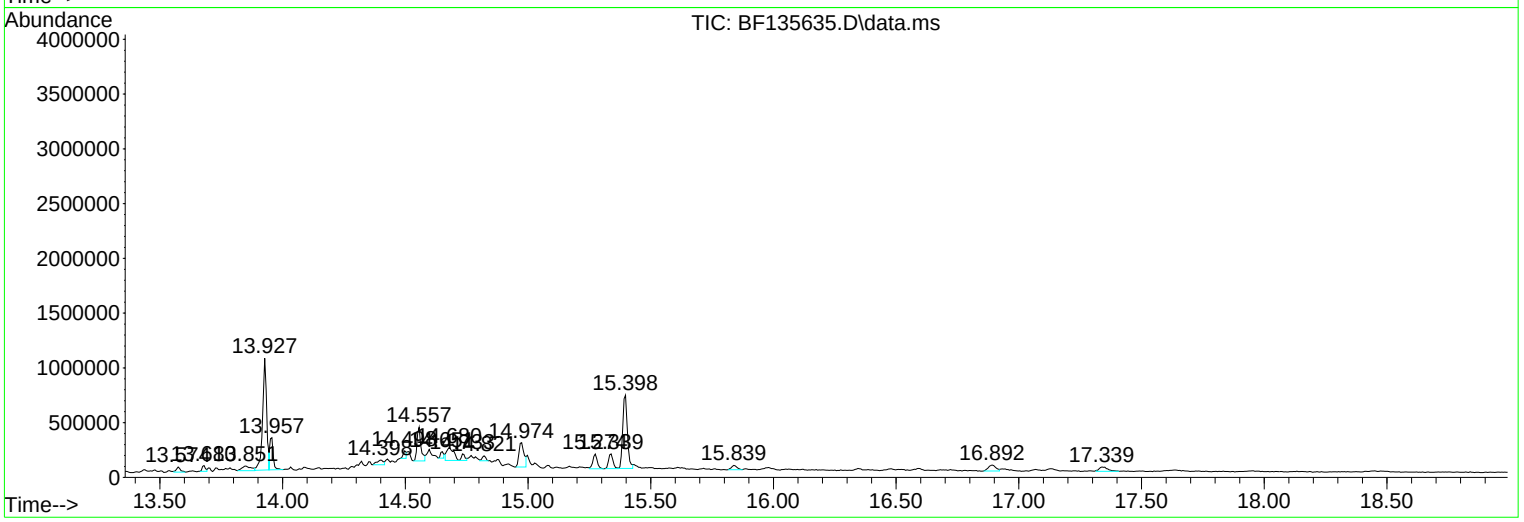
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

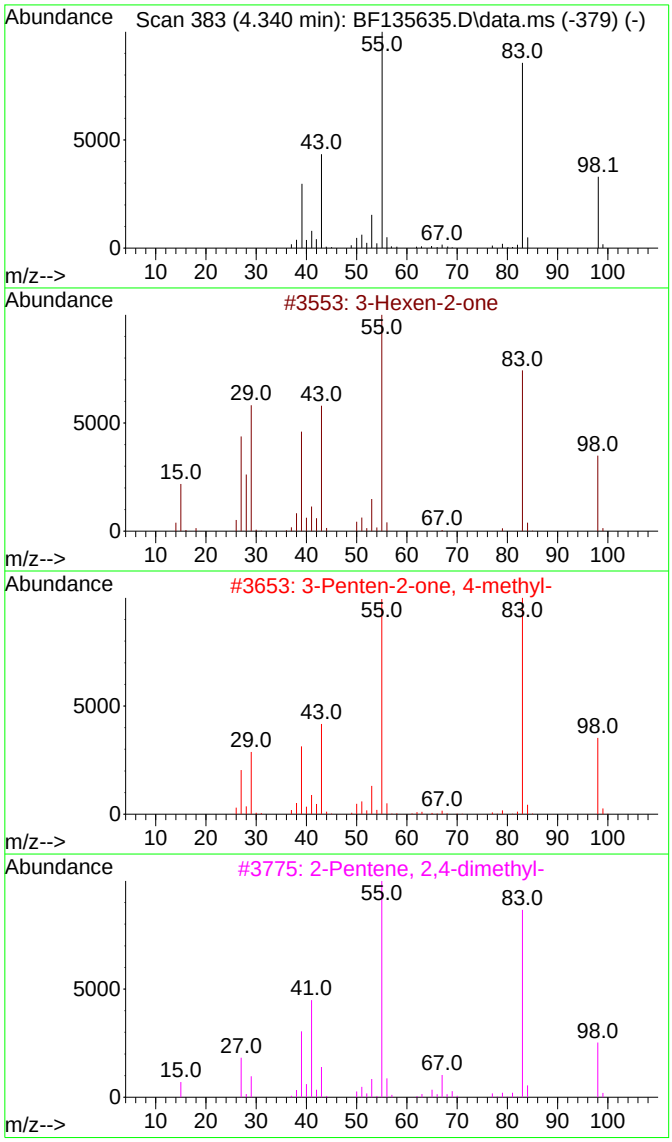
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

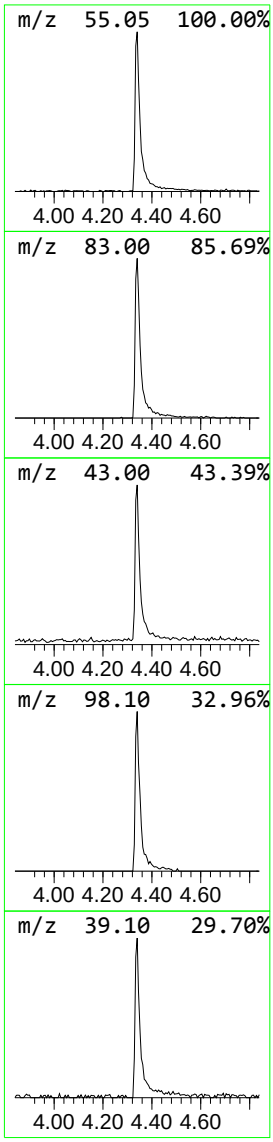
****

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	4.90 ng	233193	1,4-Dichlorobenzene-d4	6.739

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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72





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Sample : 04736-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
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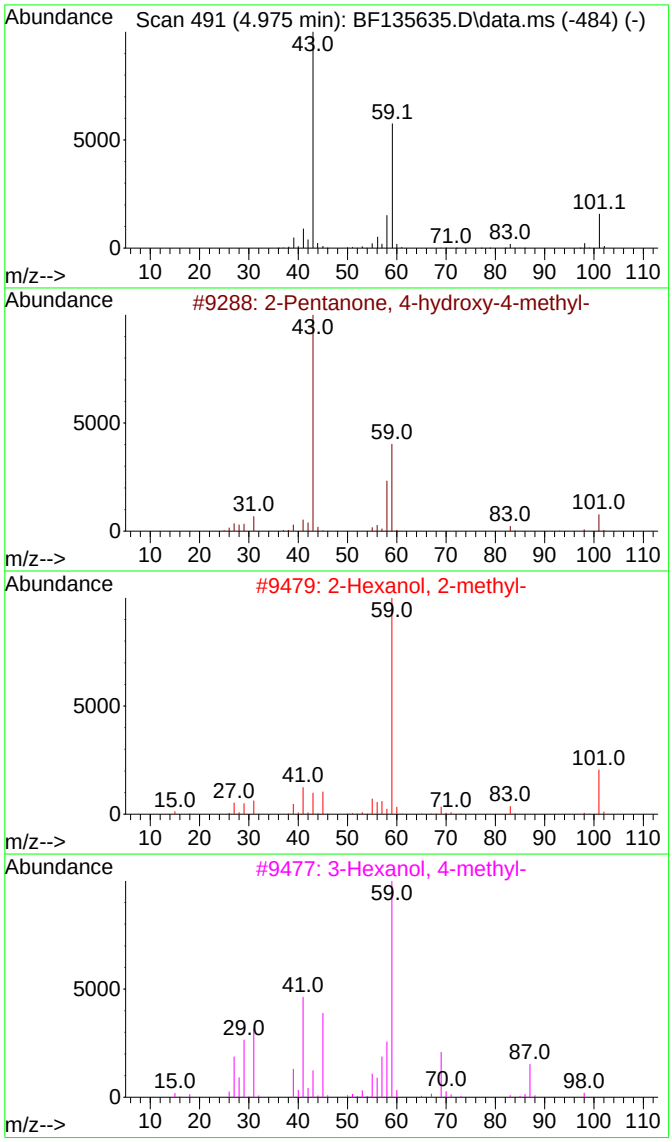
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

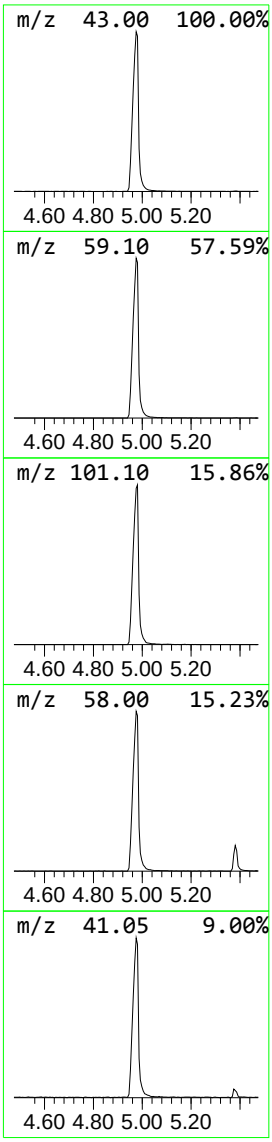
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	79.19 ng	3765870	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : 04736-02
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Instrument :
BNA_F
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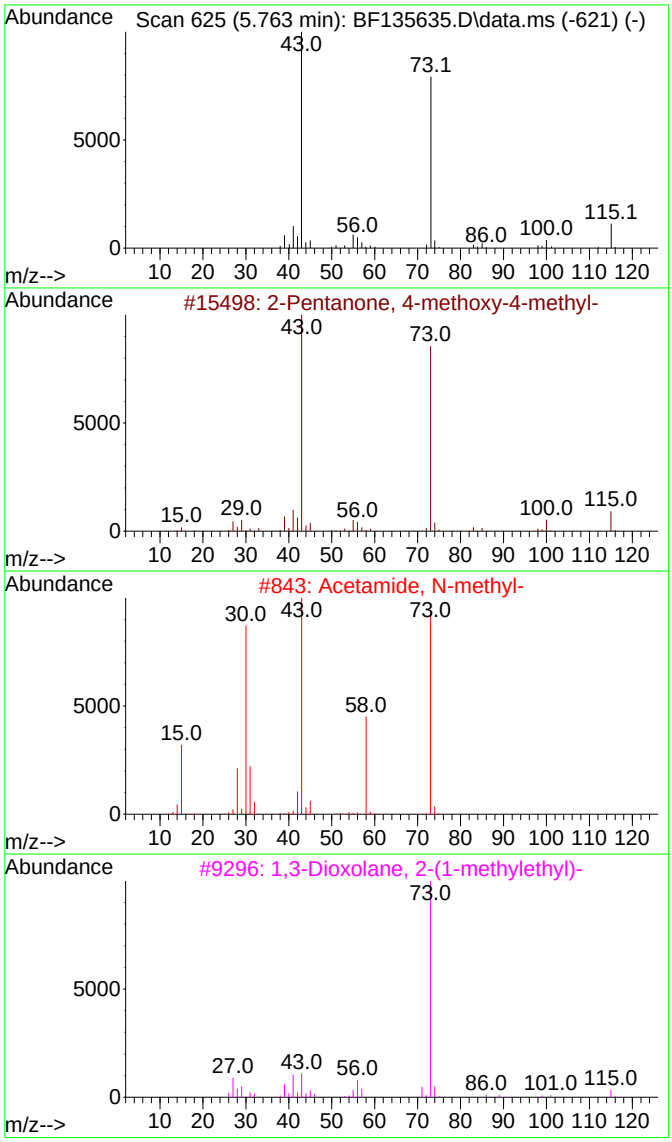
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

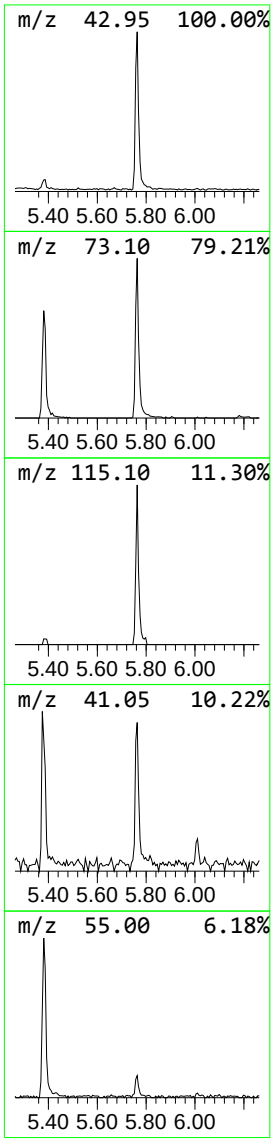
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.26 ng	107487	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4	3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
5	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	23





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

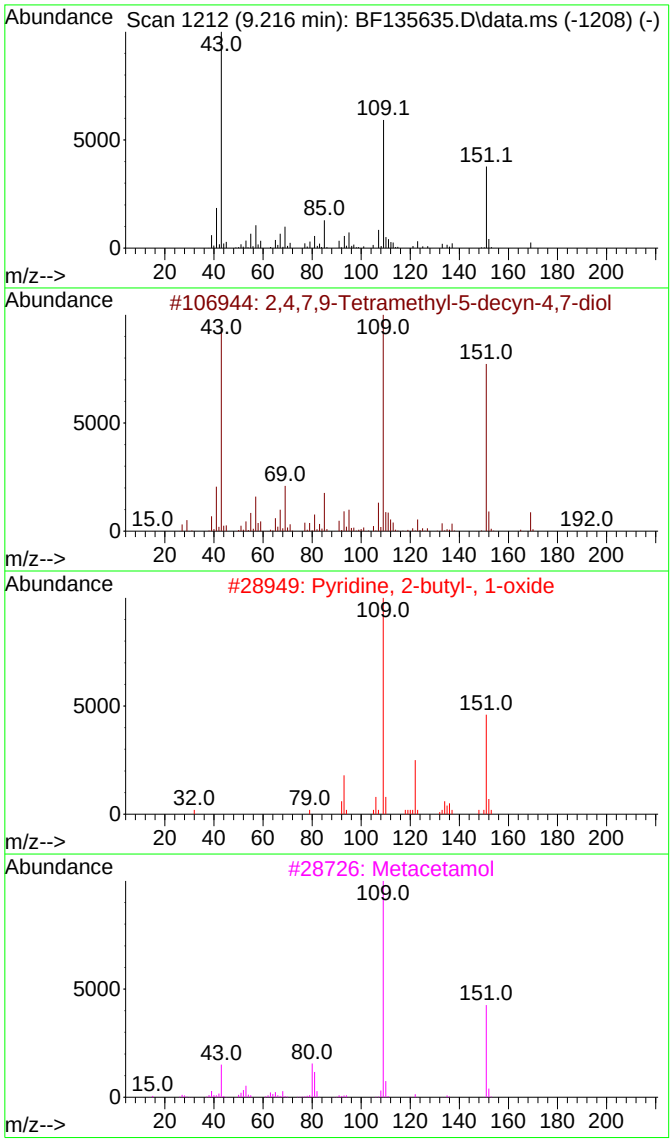
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

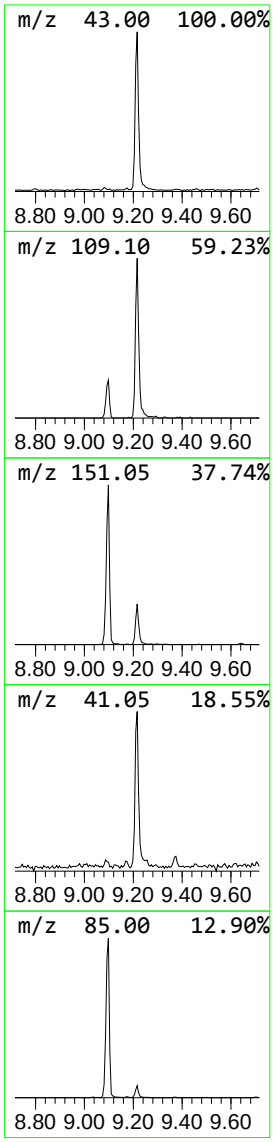
****

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	2.94 ng	201844	Acenaphthene-d10	9.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Metacetamol	151	C8H9NO2	000621-42-1	47
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

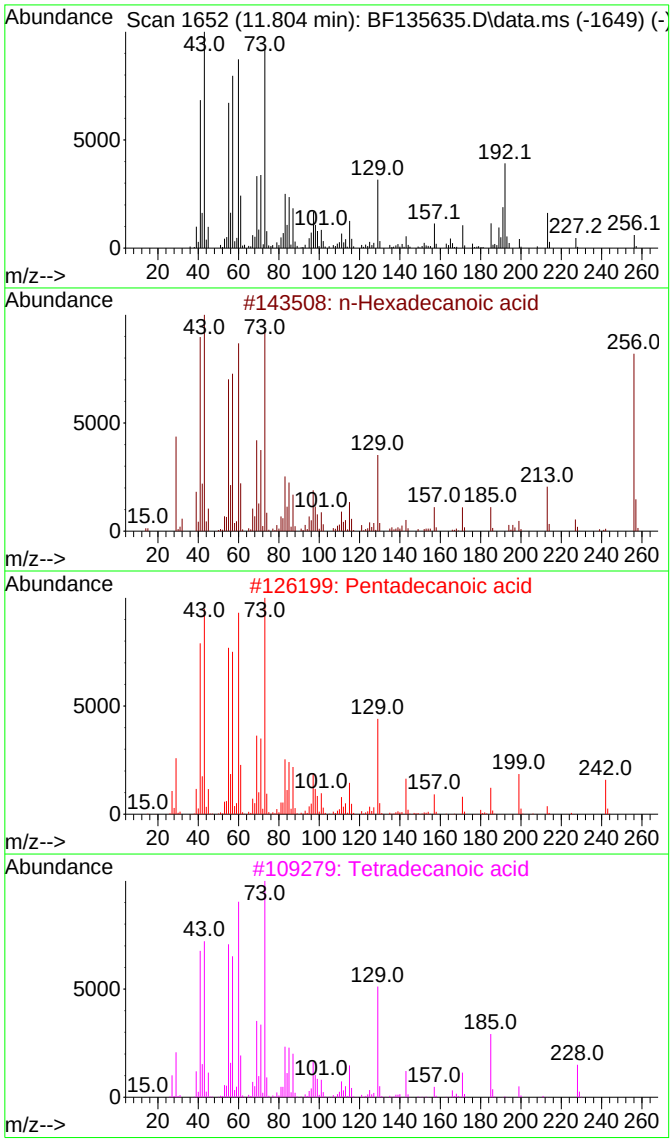
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

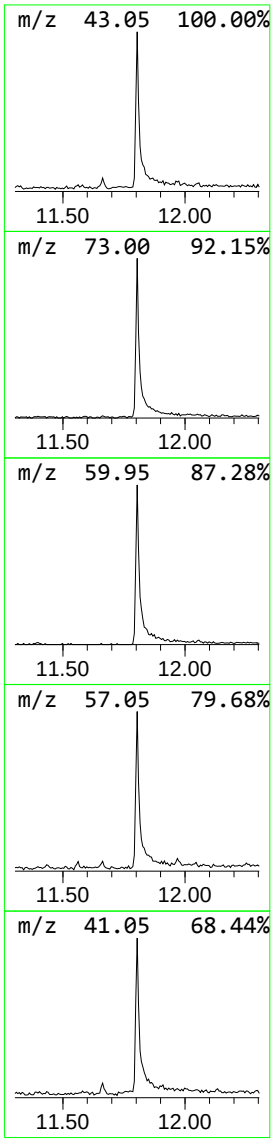
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	5.38 ng	368360	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

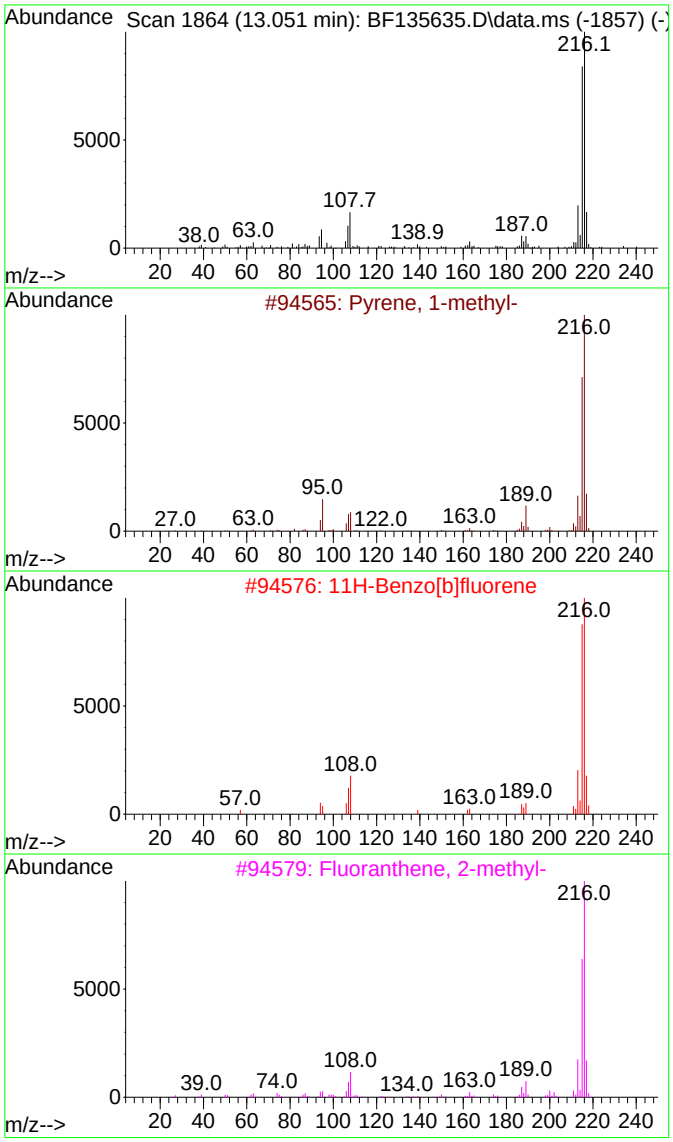
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

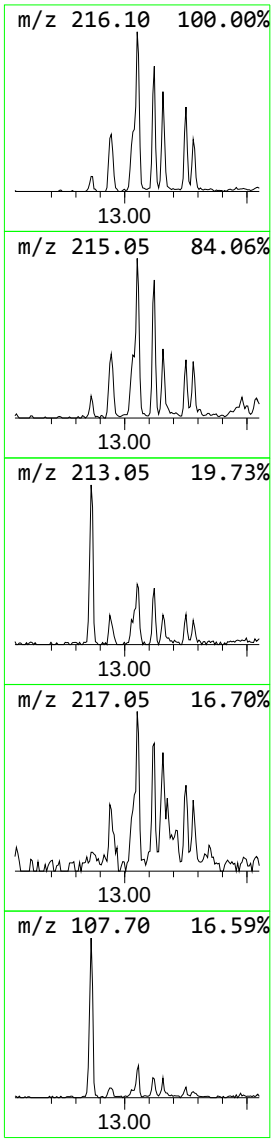
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	2.43 ng	144699	Chrysene-d12	13.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	92
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	68





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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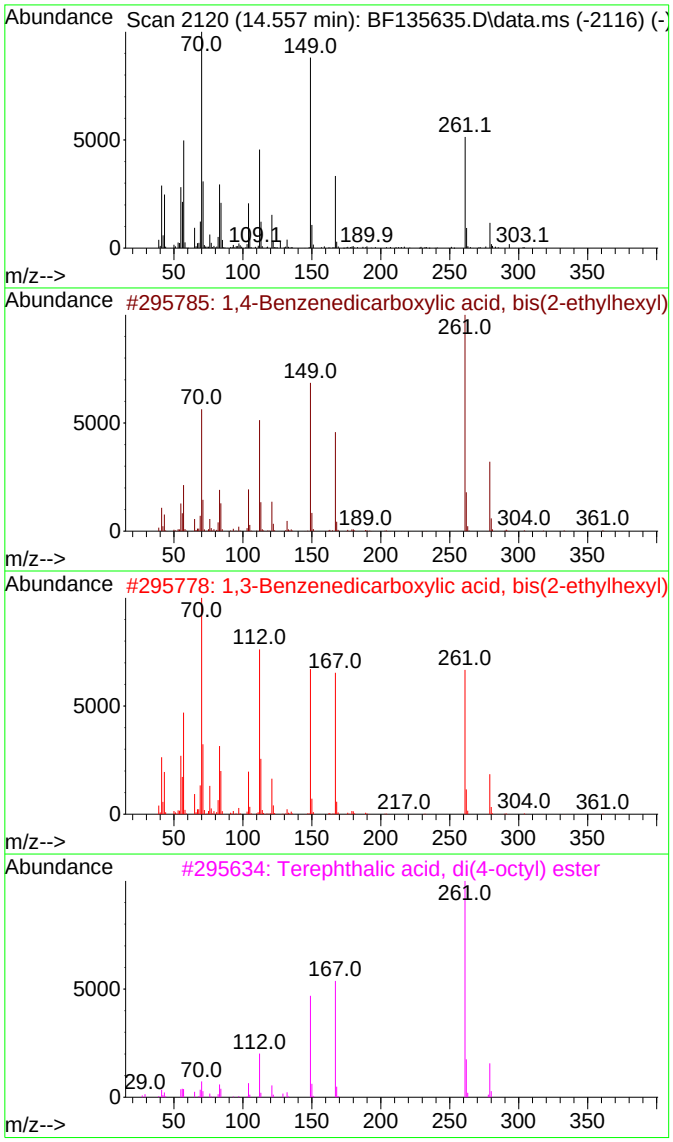
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

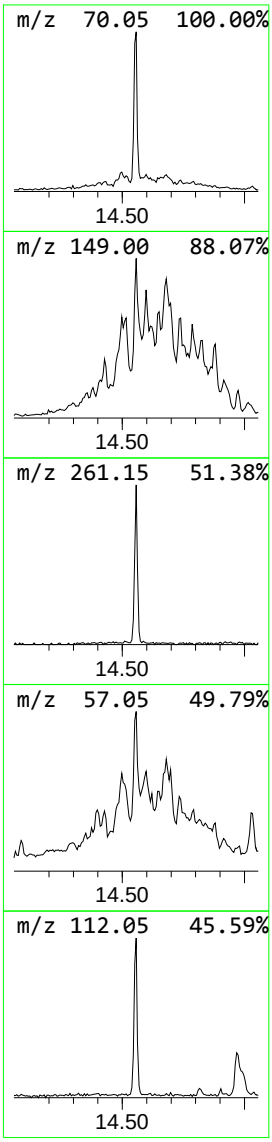
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	5.75 ng	343142	Chrysene-d12	13.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	70
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	46
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
4	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	43
5	Terephthalic acid, but-3-enyl oc...	332	C20H28O4	1000356-33-8	38





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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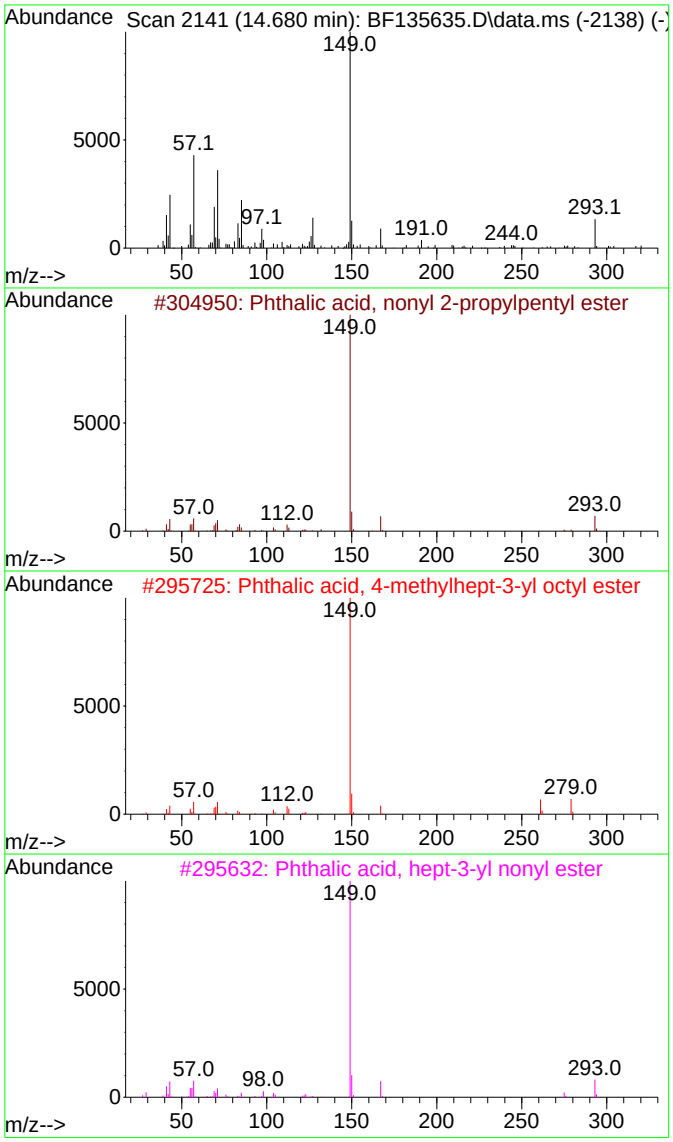
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

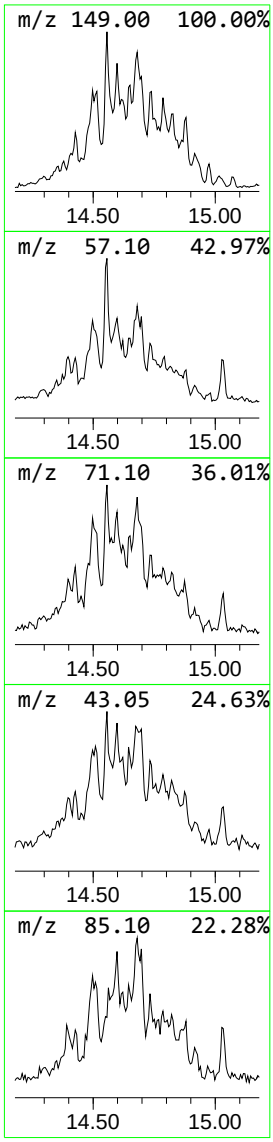
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phthalic acid, nonyl 2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.680	5.11 ng	227516	Perylene-d12	15.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, nonyl 2-propylpen...	404	C25H40O4	1000377-92-5	50
2	Phthalic acid, 4-methylhept-3-yl...	390	C24H38O4	1000377-94-3	50
3	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	50
4	Phthalic acid, 5-methylhex-2-yl ...	390	C24H38O4	1000371-08-5	50
5	Phthalic acid, 3,3-dimethylbut-2...	306	C18H26O4	1000357-00-1	50





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Acq On : 06 Oct 2023 18:25
Operator : CG\JU
Sample : 04736-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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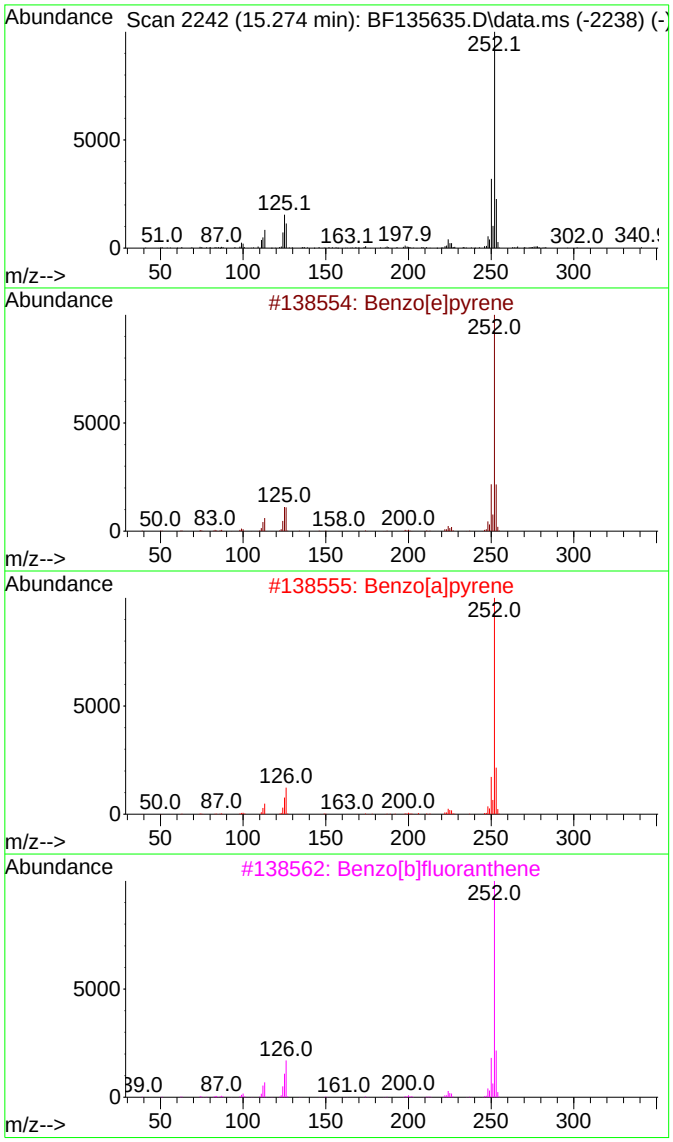
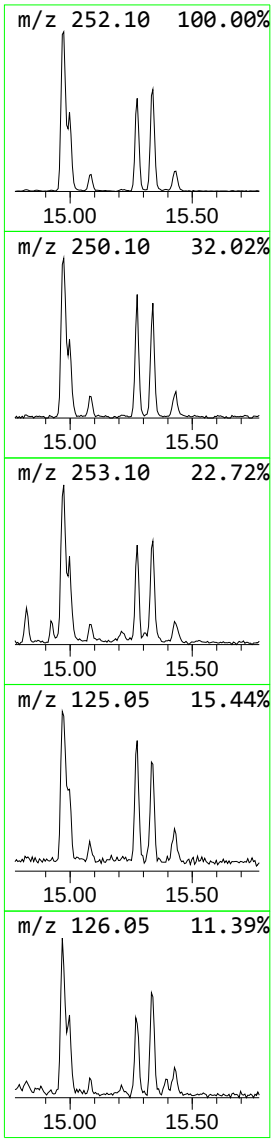
Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	3.71 ng	164946	Perylene-d12	15.398

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





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Data File : BF135635.D
Acq On : 06 Oct 2023 18:25
Operator : CG\JU
Sample : 04736-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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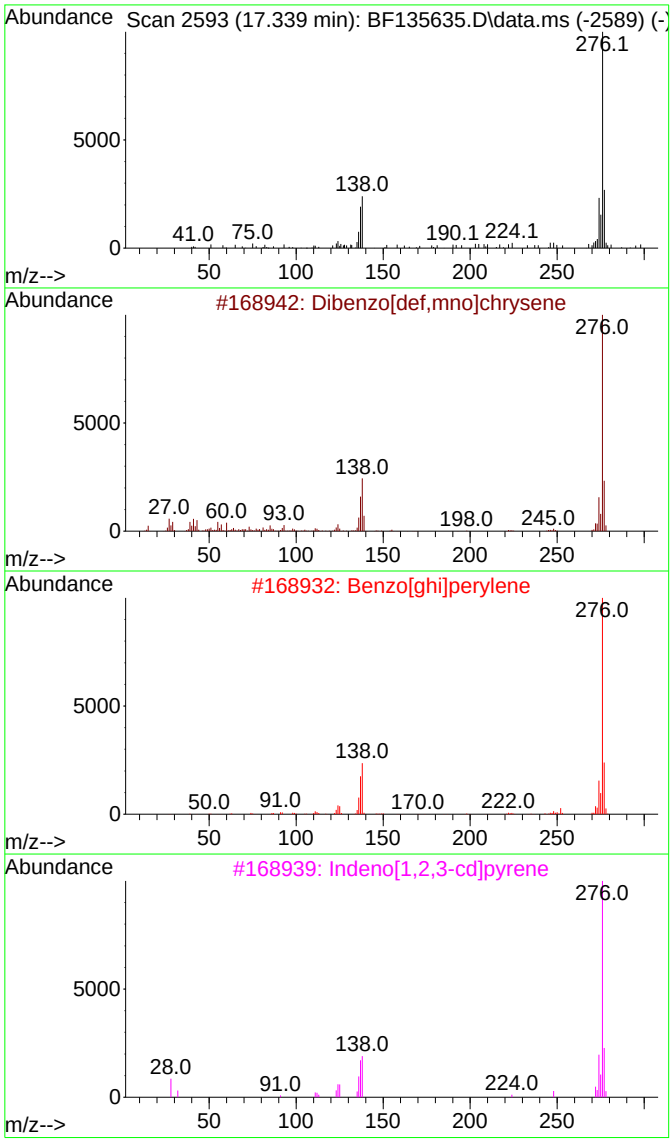
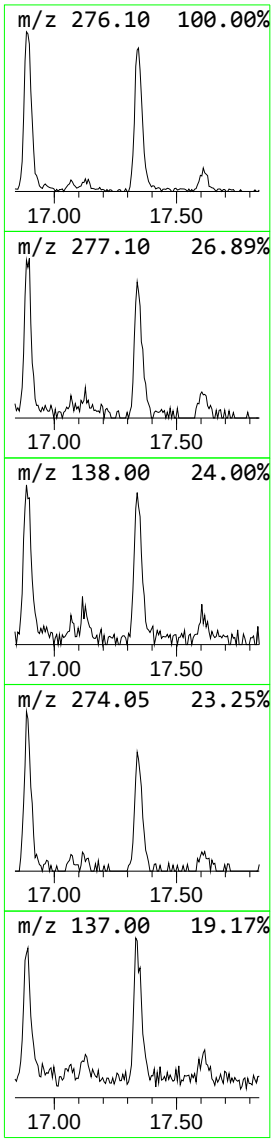
Peak Number 11 Dibenzo[def,mno]chrysene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	2.17 ng	96775	Perylene-d12	15.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	94
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	93
3	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	72
5	Phosphoric acid, 4-methoxy-2-(me...	276	C11H17O6P	094420-71-0	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135635.D
Acq On : 06 Oct 2023 18:25
Operator : CG\JU
Sample : 04736-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
3-Hexen-2-one	4.340	4.9	ng	233193	1	6.739	951090	20.0
2-Pentanone, 4-...	4.975	79.2	ng	3765870	1	6.739	951090	20.0
2-Pentanone, 4-...	5.763	2.3	ng	107487	1	6.739	951090	20.0
2,4,7,9-Tetrame...	9.216	2.9	ng	201844	3	9.775	1371840	20.0
n-Hexadecanoic ...	11.804	5.4	ng	368360	4	11.269	1368880	20.0
Pyrene, 1-methyl-	13.051	2.4	ng	144699	5	13.927	1192520	20.0
1,4-Benzenedica...	14.557	5.8	ng	343142	5	13.927	1192520	20.0
Phthalic acid, ...	14.680	5.1	ng	227516	6	15.398	890208	20.0
Benzo[e]pyrene	15.274	3.7	ng	164946	6	15.398	890208	20.0
Dibenzo[def,mno...	17.339	2.2	ng	96775	6	15.398	890208	20.0