LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132489.D
Acq On : 20 Feb 2023 20:43
Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

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-BF021623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.260	408	412	427	rVB	1521850	1962613	48.06%	5.234%
2	5.654	474	479	482	rBV	4291375	4084050	100.00%	10.891%
3	6.654	644	649	652	rBV	3945490	4035953	98.82%	10.763%
4	7.031	709	713	716	rBV	1182830	1038752	25.43%	2.770%
5	7.589	804	808	811	rBV	2777934	2500402	61.22%	6.668%
6	8.313	928	931	934	rBV	1479312	1207440	29.56%	3.220%
7	8.336	934	935	937	rVB	153179	70626	1.73%	0.188%
8	9.031	1049	1053	1055	rVB	62661	53127	1.30%	0.142%
9	9.389	1110	1114	1117	rBV	4884281	3990567	97.71%	10.642%
10	9.460	1123	1126	1129	rBV	62607	63268	1.55%	0.169%
11	9.654	1155	1159	1165	rBV2	33152	49705	1.22%	0.133%
12	9.731	1168	1172	1175	rBV3	42697	47195	1.16%	0.126%
13	9.936	1204	1207	1212	rBV	103395	92053	2.25%	0.245%
14	9.989	1213	1216	1218	rVB	69541	54775	1.34%	0.146%
15	10.078	1228	1231	1234	rVB	1435708	1089269	26.67%	2.905%
16	10.107	1234	1236	1240	rVB	202269	174249	4.27%	0.465%
17	10.283	1262	1266	1269	rVB	121786	116083	2.84%	0.310%
18	10.489	1298	1301	1304	rVB2	64232	61755	1.51%	0.165%
19	10.625	1321	1324	1329	rVB	153937	145155	3.55%	0.387%
20	10.730	1340	1342	1345	rVB	252402	192882	4.72%	0.514%
21	10.789	1349	1352	1355	rVB	153110	135754	3.32%	0.362%
22	10.872	1362	1366	1369	rBV	2394688	2071804	50.73%	5.525%
23	10.977	1379	1384	1392	rVB3	97711	163439	4.00%	0.436%
24	11.307	1435	1440	1441	rBV3	35480	57763	1.41%	0.154%
25	11.419	1456	1459	1462	rBV2	89407	105773	2.59%	0.282%
26	11.472	1466	1468	1471	rVB	97845	76521	1.87%	0.204%
27	11.577	1482	1486	1488	rBV	1127952	1177879	28.84%	3.141%
28	11.601	1488	1490	1493	rVB	1194417	940530	23.03%	2.508%
29	11.648	1493	1498	1501	rBV	446428	402649	9.86%	1.074%
30	11.683	1501	1504	1507	rVB2	66521	65256	1.60%	0.174%
31	11.801	1521	1524	1529	rBV2	130486	156231	3.83%	0.417%
32	12.077	1568	1571	1574	rBV2	310646	342838	8.39%	0.914%
33	12.107	1574	1576	1580	rVB2	255106	206742	5.06%	0.551%
34	12.154	1582	1584	1587	rVB	123867	97996	2.40%	0.261%
35	12.195	1587	1591	1593	rBV2	368212	377408	9.24%	1.006%
36	12.254	1599	1601	1604	rBV2	80234	77665	1.90%	0.207%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
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Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

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-BF021623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.372	1619	1621	1624	rBV	145079	137784	3.37%	0.367%
38	12.401	1624	1626	1629	rVV2	75804	63753	1.56%	0.170%
39	12.630	1662	1665	1667	rBV	136395	152657	3.74%	0.407%
40	12.801	1690	1694	1697	rBV	2205789	1956249	47.90%	5.217%
41	13.030	1727	1733	1739	rBV	1869460	2243128	54.92%	5.982%
42	13.166	1752	1756	1759	rBV	3582565	3018860	73.92%	8.051%
43	13.360	1786	1789	1791	rVB	270541	259885	6.36%	0.693%
44	13.424	1798	1800	1802	rVB	283661	208759	5.11%	0.557%
45	14.230	1934	1937	1941	rBV2	948340	1399133	34.26%	3.731%
46	14.266	1941	1943	1948	rVB	655680	571597	14.00%	1.524%

Sum of corrected areas: 37497972

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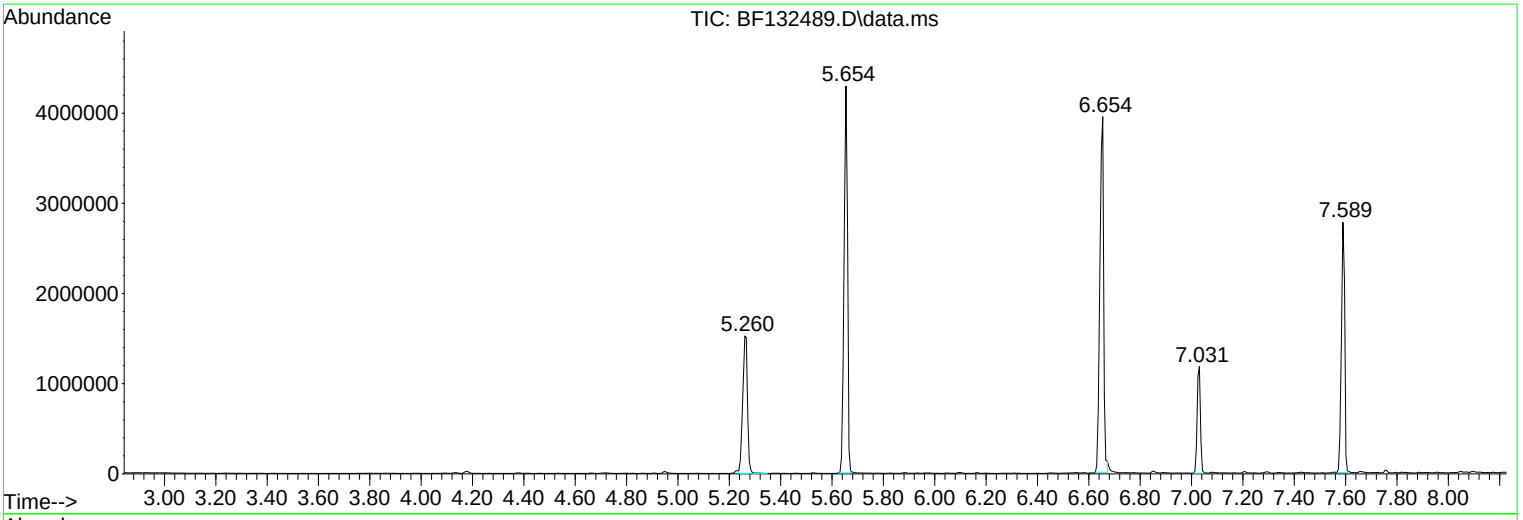
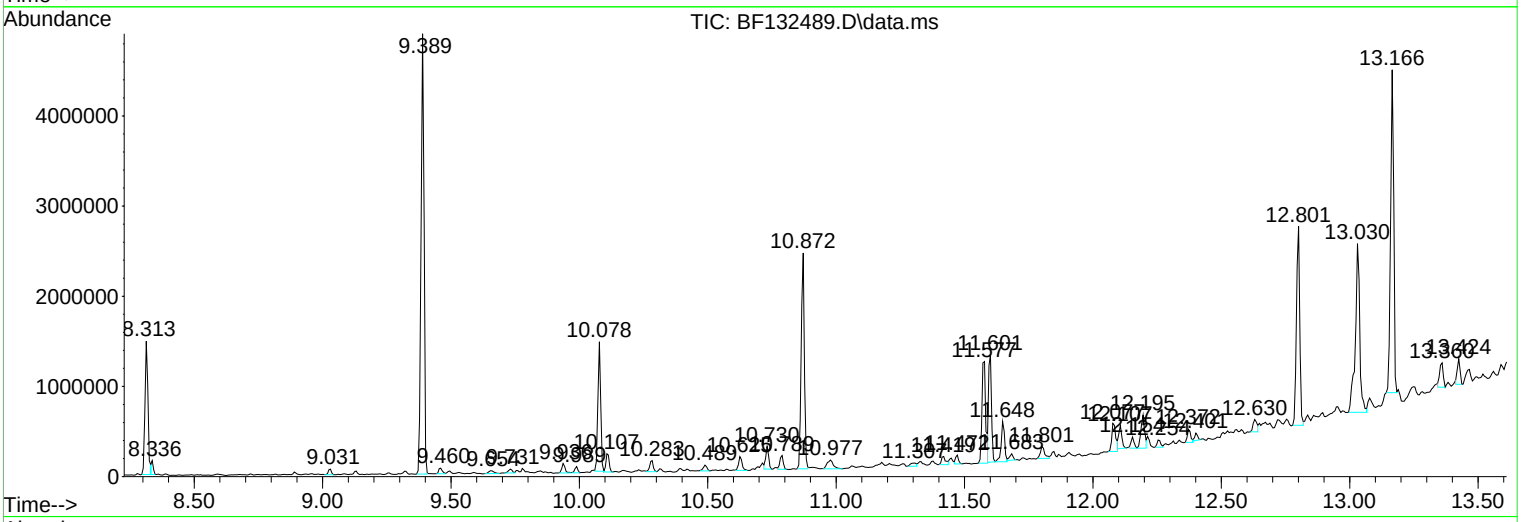
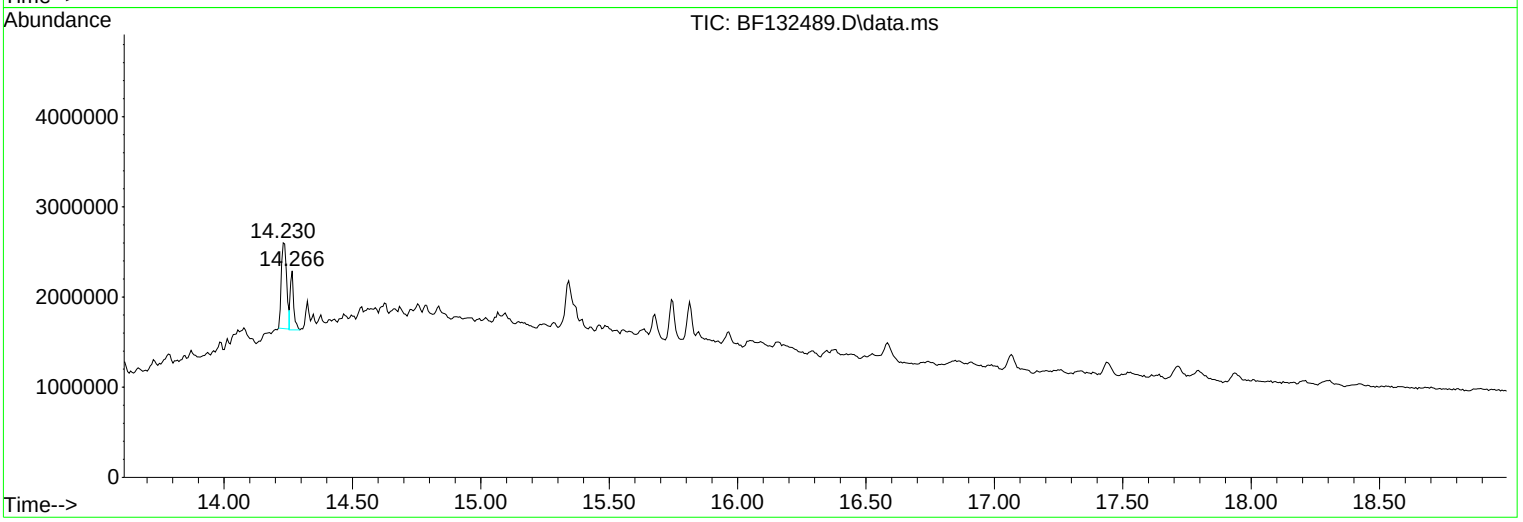
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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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Data File : BF132489.D
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Instrument :
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SB-06-0-2.0

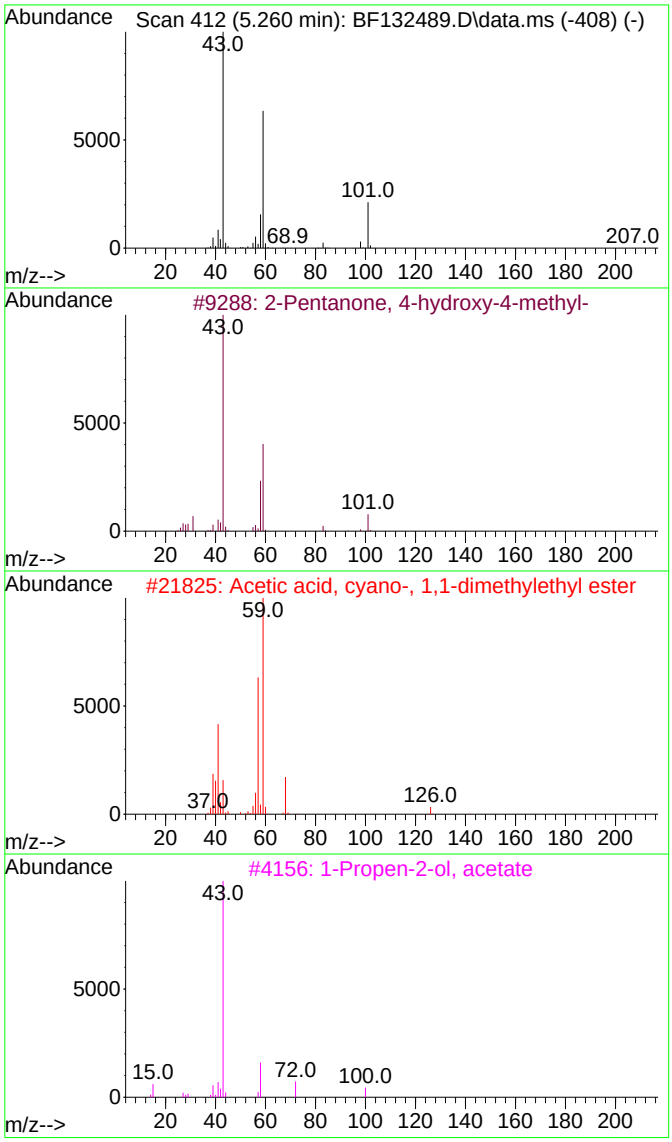
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

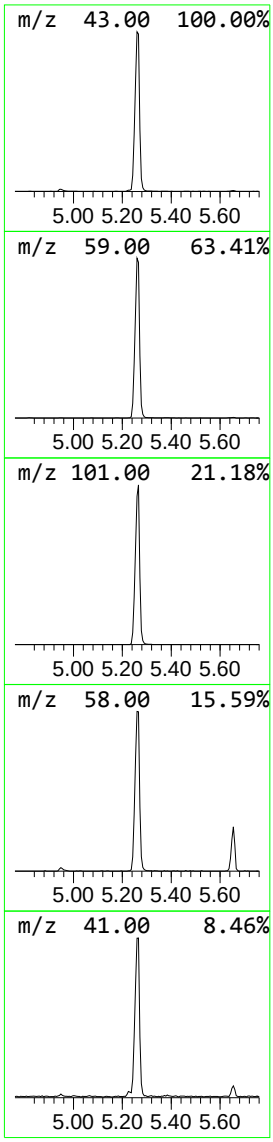
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.260	37.79 ng	1962610	1,4-Dichlorobenzene-d4	7.031

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Operator : CG\JU
Sample : 01552-11
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Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

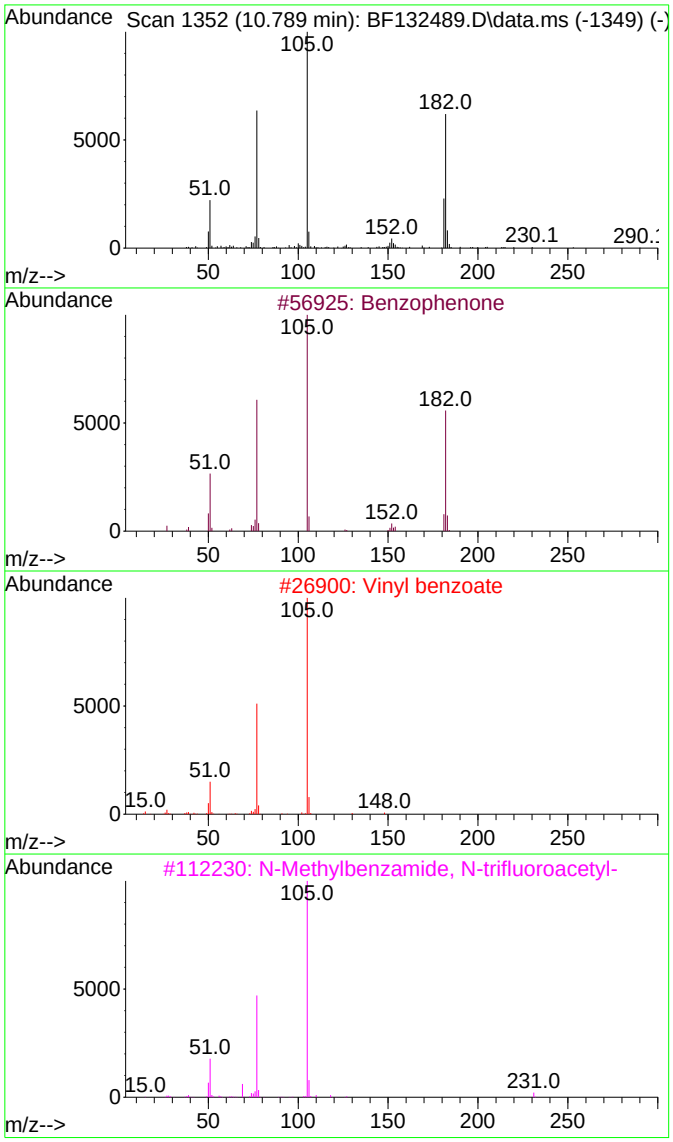
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

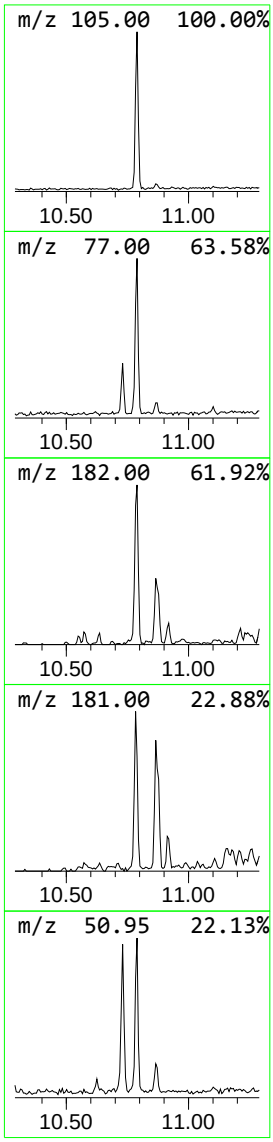
****

Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.789	2.49 ng	135754	Acenaphthene-d10	10.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Vinyl benzoate	148	C9H8O2	000769-78-8	46
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43
4	2-Pyrazoline-3-carbonitrile, 1-b...	199	C11H9N3O	067872-68-8	43
5	N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2NO3S	136800-77-6	43





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Operator : CG\JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

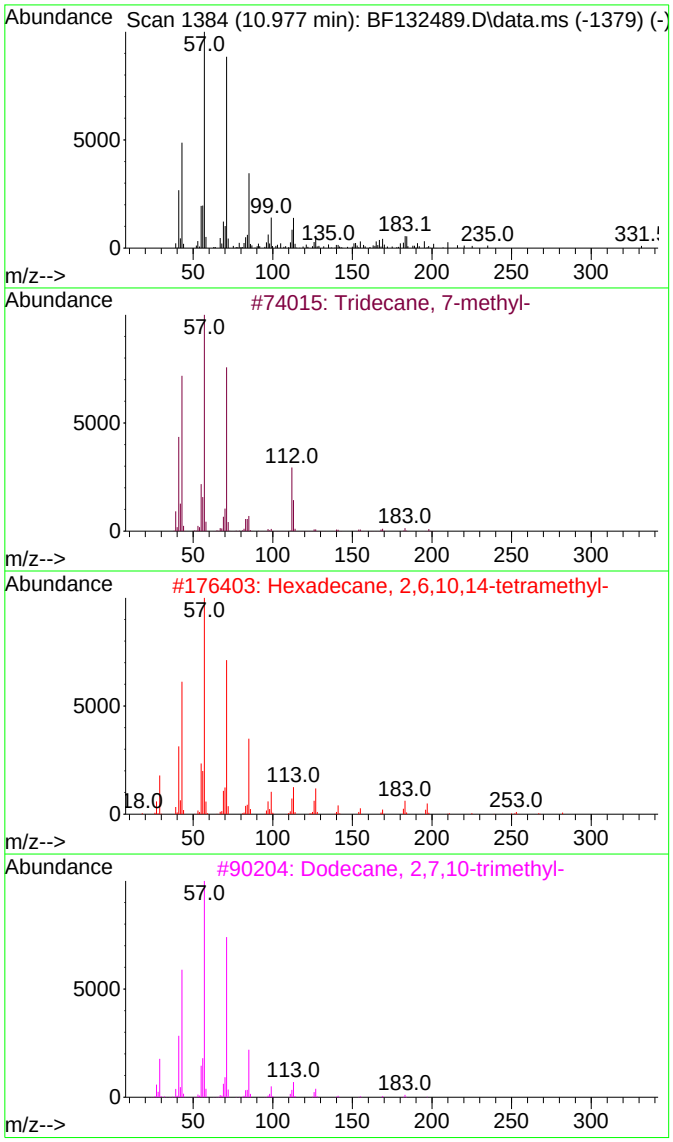
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

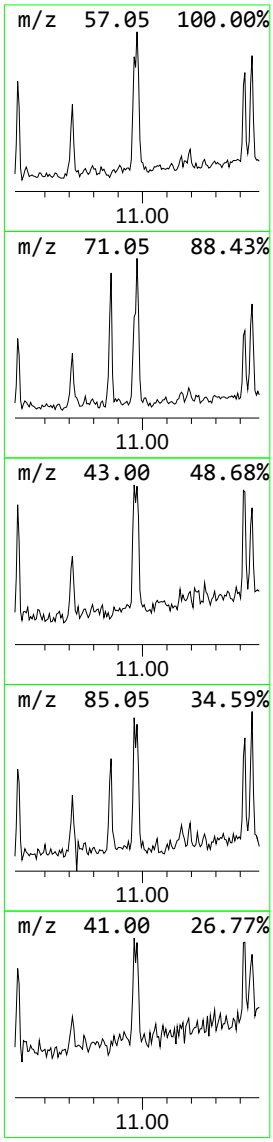
****

Peak Number 4 Tridecane, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.977	2.78 ng	163439	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	89
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	80
5	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

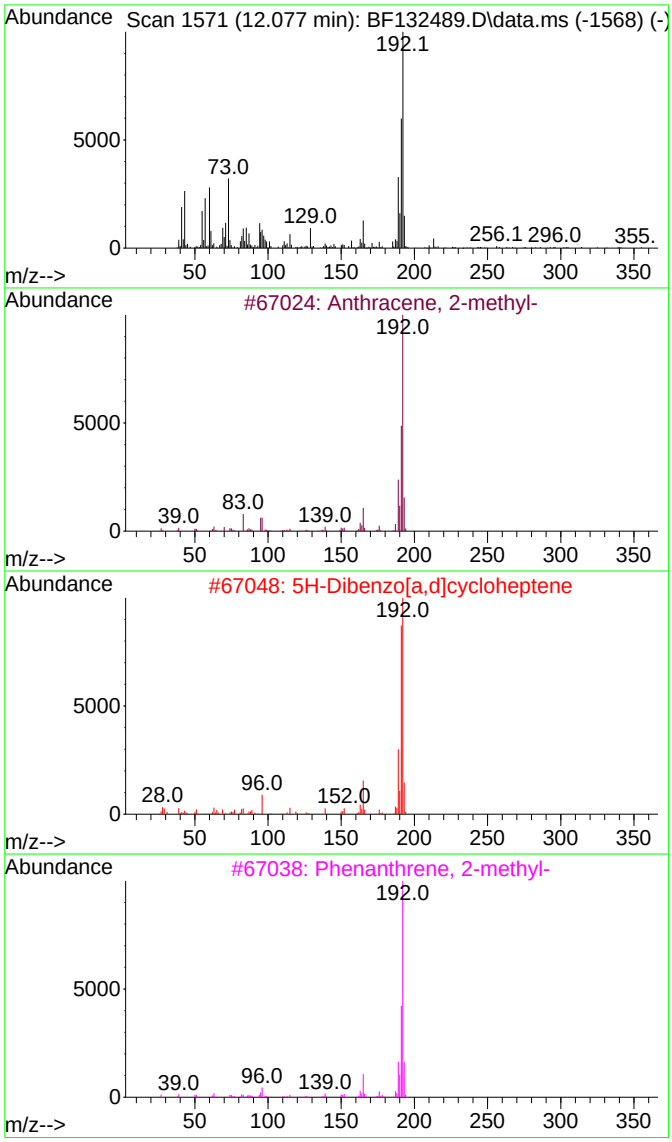
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

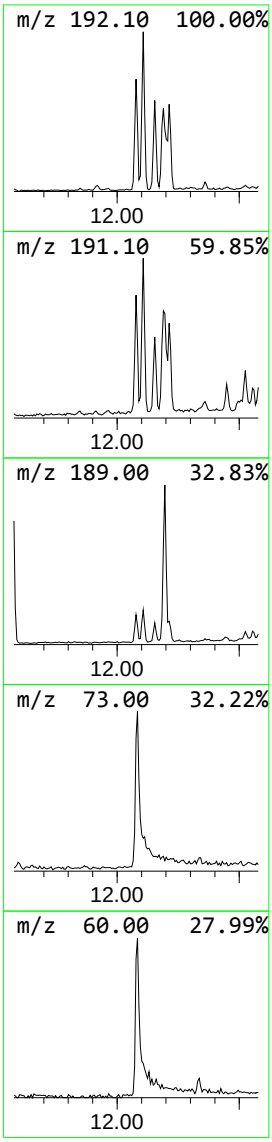
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.077	5.82 ng	342838	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	91
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	86





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BNA_F
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SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

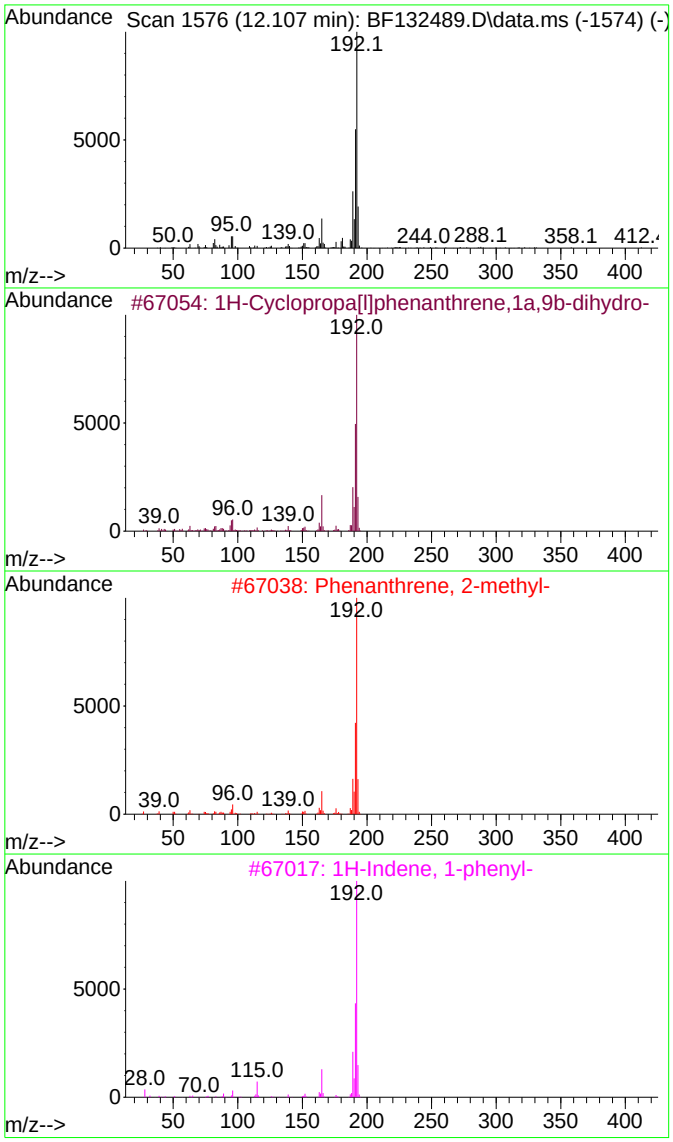
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

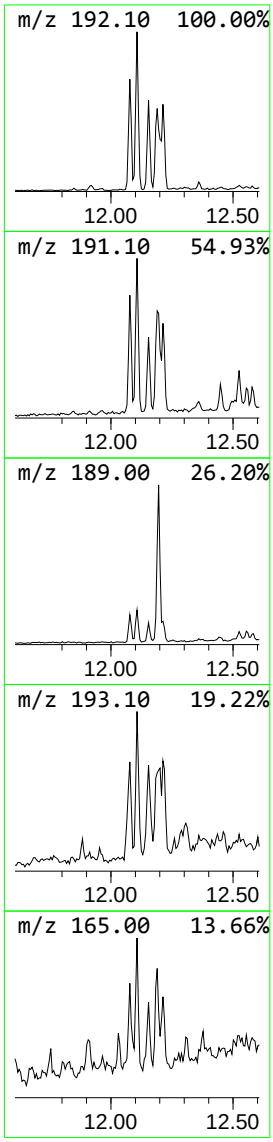
****

Peak Number 6 1H-Cyclopropa[l]phenanthren... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.107	3.51 ng	206742	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	94
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

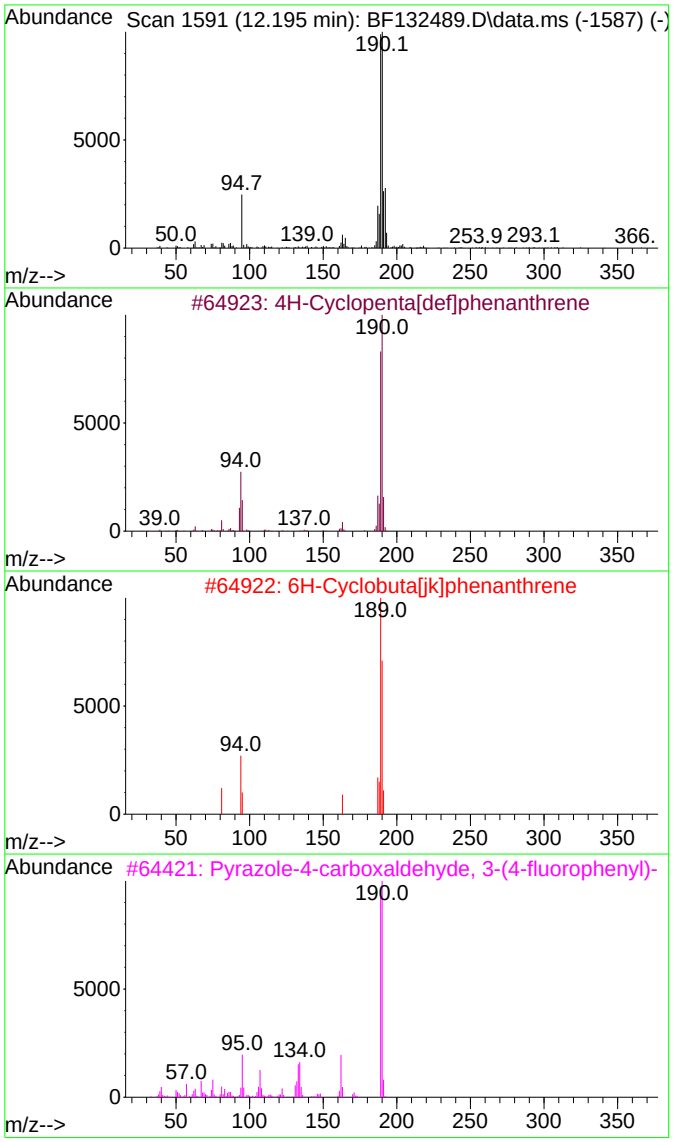
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

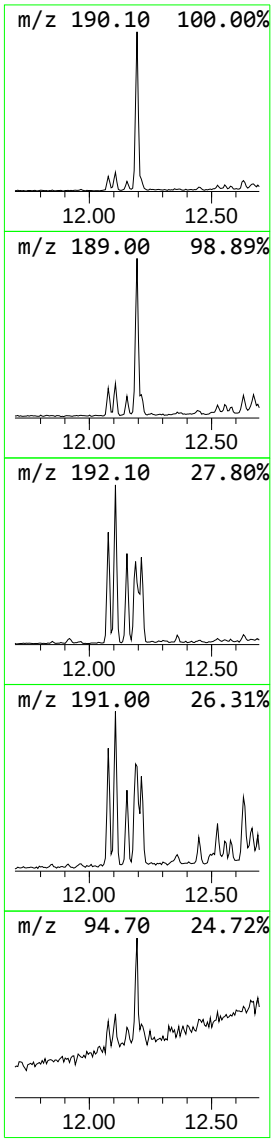
****

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.195	6.41 ng	377408	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	17





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ClientSampleId :
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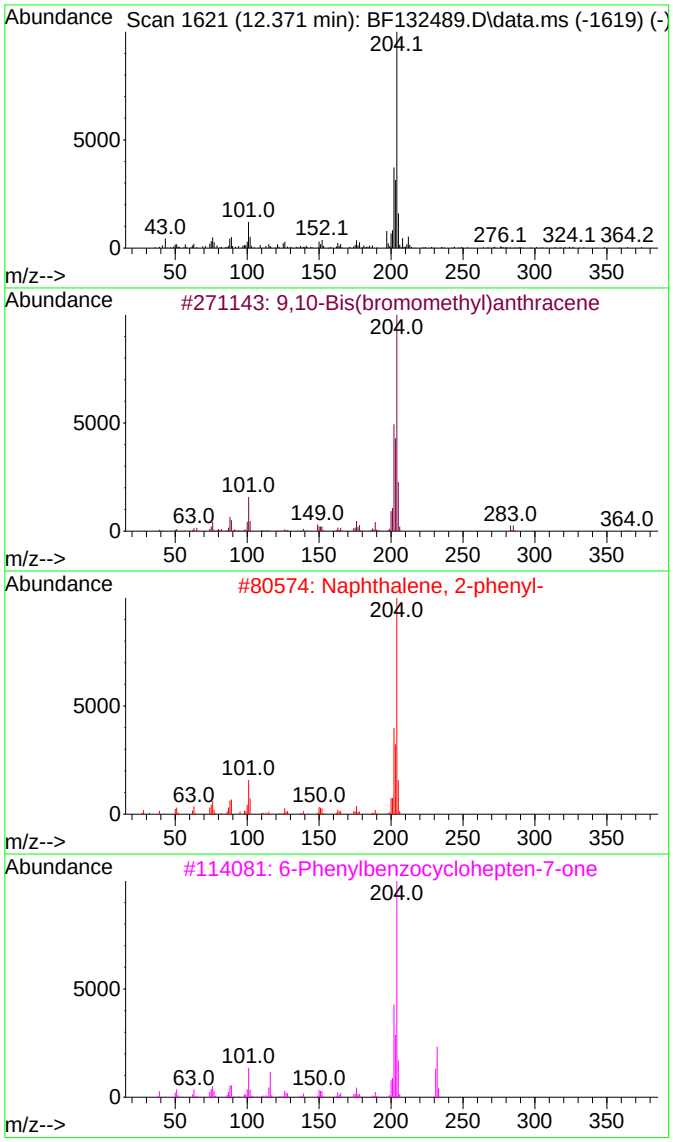
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

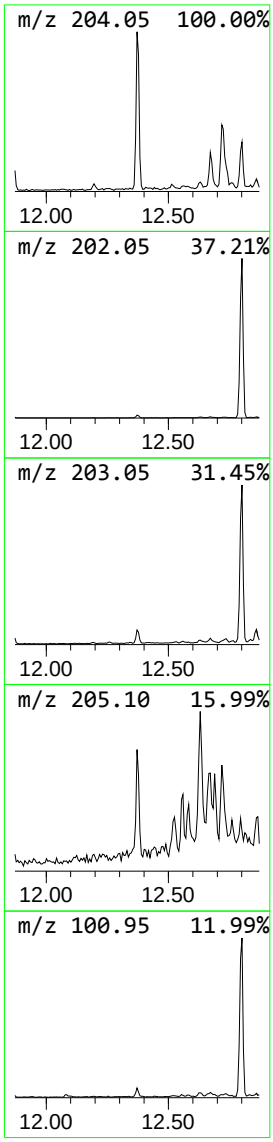
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9,10-Bis(bromomethyl)anthra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.371	2.34 ng	137784	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	98
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	93
3	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	87
4	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	86
5	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132489.D
Acq On : 20 Feb 2023 20:43
Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

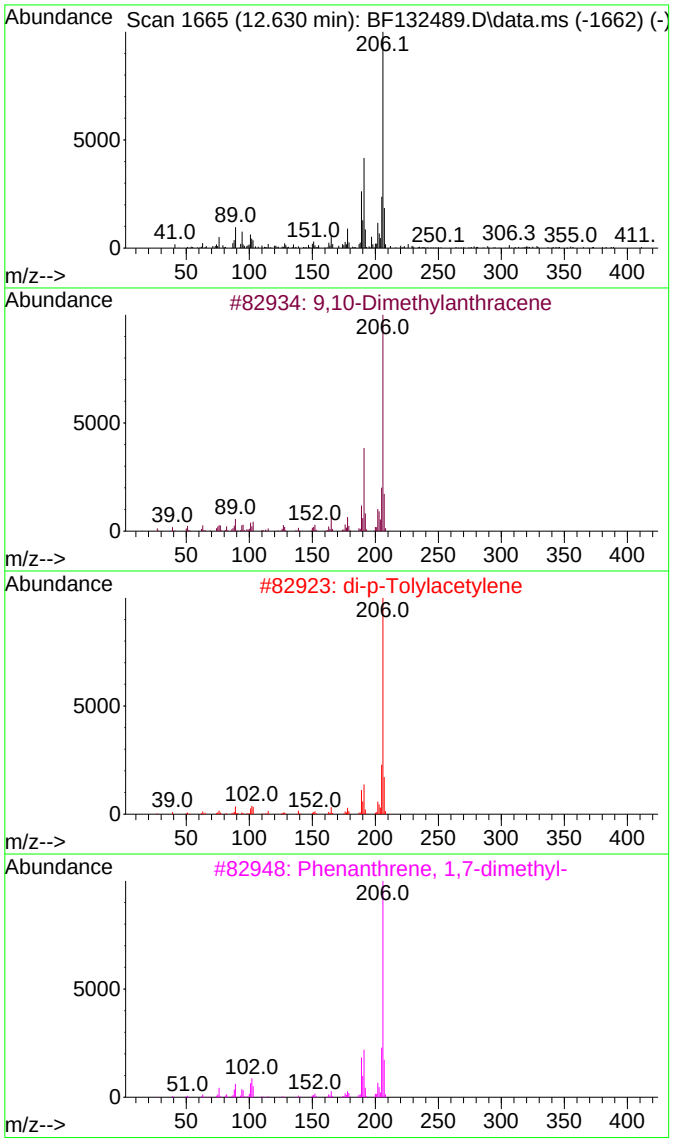
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

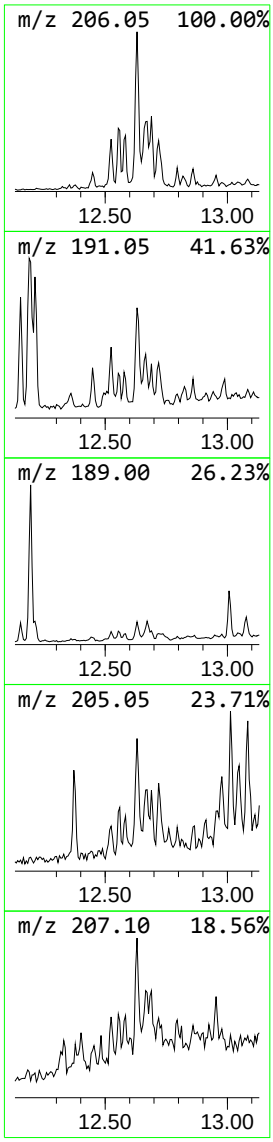
****

Peak Number 9 9,10-Dimethylanthracene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.630	2.59 ng	152657	Phenanthrene-d10	11.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	94
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	94
3	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93





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Data File : BF132489.D
Acq On : 20 Feb 2023 20:43
Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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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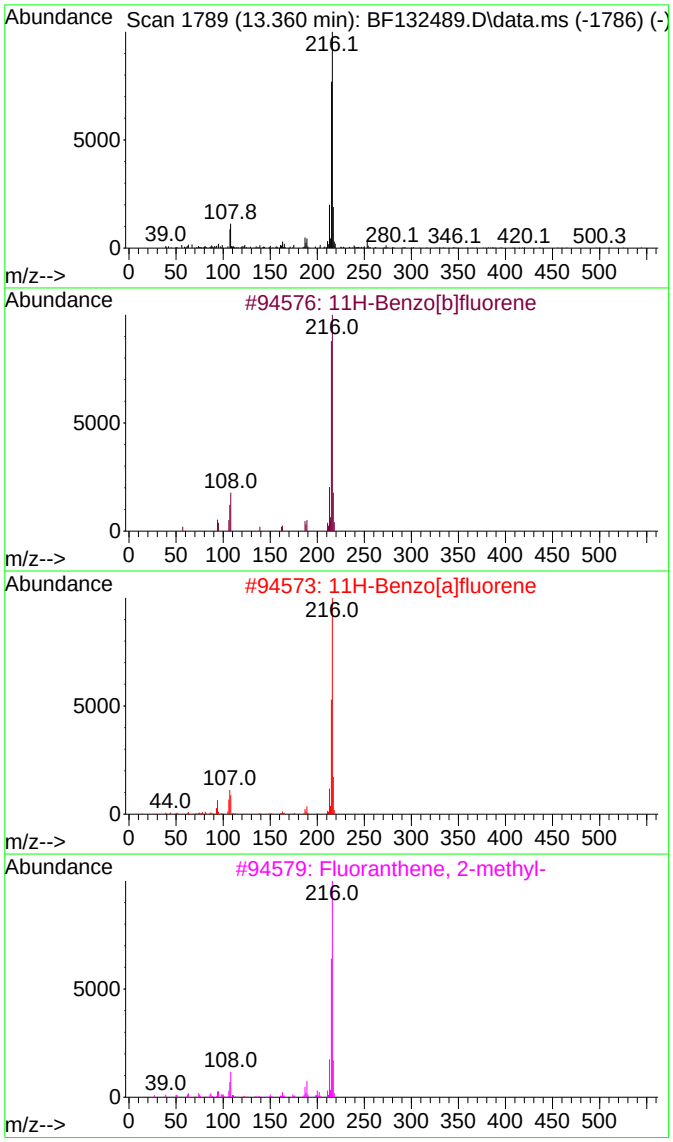
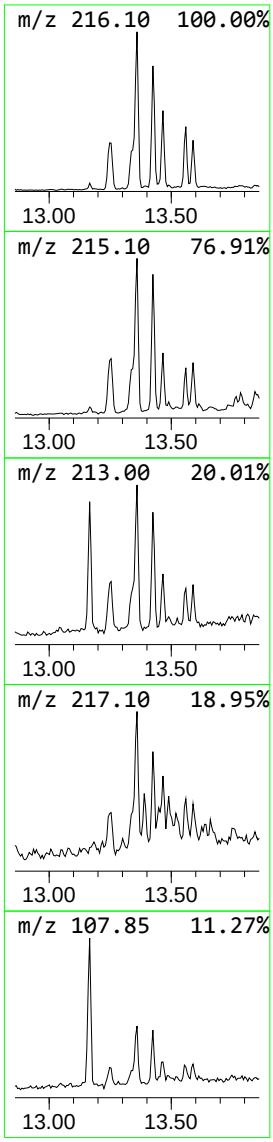
Peak Number 10 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.360	3.71 ng	259885	Chrysene-d12	14.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	72





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Data File : BF132489.D
Acq On : 20 Feb 2023 20:43
Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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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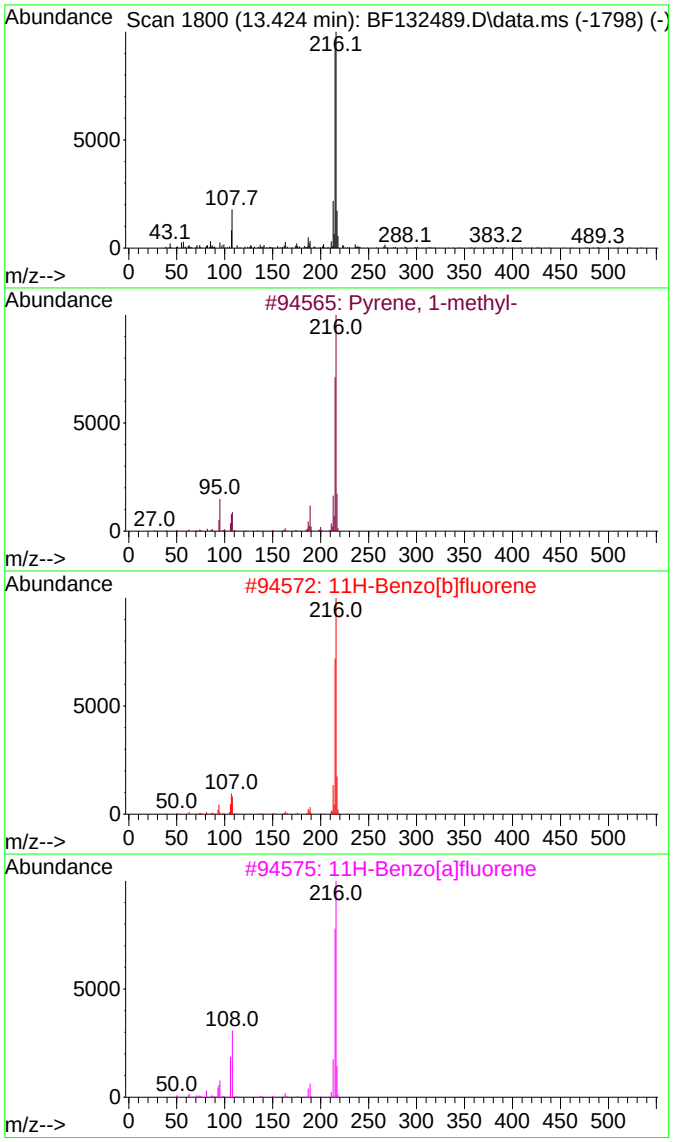
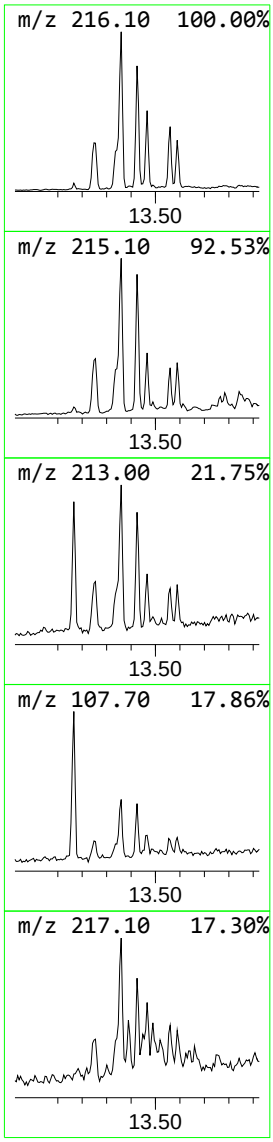
Peak Number 11 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.424	2.98 ng	208759	Chrysene-d12	14.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132489.D
Acq On : 20 Feb 2023 20:43
Operator : CG\JU
Sample : 01552-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-...	5.260	37.8	ng	1962610	1	7.031	1038750	20.0
Benzophenone	10.789	2.5	ng	135754	3	10.078	1089270	20.0
Tridecane, 7-me...	10.977	2.8	ng	163439	4	11.577	1177880	20.0
Anthracene, 2-m...	12.077	5.8	ng	342838	4	11.577	1177880	20.0
1H-Cyclopropa[l...	12.107	3.5	ng	206742	4	11.577	1177880	20.0
4H-Cyclopenta[d...	12.195	6.4	ng	377408	4	11.577	1177880	20.0
9,10-Bis(bromom...	12.371	2.3	ng	137784	4	11.577	1177880	20.0
9,10-Dimethylan...	12.630	2.6	ng	152657	4	11.577	1177880	20.0
11H-Benzo[b]flu...	13.360	3.7	ng	259885	5	14.236	1399130	20.0
Pyrene, 1-methyl-	13.424	3.0	ng	208759	5	14.236	1399130	20.0