LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	15	24	rVB	938070	1477191	38.26%	4.351%
2	5.104	500	512	520	rBV	63813	104127	2.70%	0.307%
3	5.504	574	580	601	rBV	2226294	2938349	76.11%	8.654%
4	6.510	745	751	779	rBV	2314498	3228833	83.64%	9.509%
5	6.869	807	812	818	rBV	704814	879593	22.78%	2.591%
6	7.433	901	908	918	rBV	1571246	2139889	55.43%	6.302%
7	7.681	945	950	961	rBV	33389	52694	1.36%	0.155%
8	8.151	1022	1030	1048	rBV	897208	1184209	30.67%	3.488%
9	9.227	1206	1213	1223	rBV	2891872	3860618	100.00%	11.370%
10	9.904	1322	1328	1333	rBV	1010462	1345291	34.85%	3.962%
11	9.939	1333	1334	1339	rVB	67275	51286	1.33%	0.151%
12	10.110	1358	1363	1367	rBV	34289	48043	1.24%	0.141%
13	10.457	1415	1422	1427	rBV	53139	72968	1.89%	0.215%
14	10.621	1444	1450	1457	rVB	334481	438701	11.36%	1.292%
15	10.698	1457	1463	1478	rVV	1704054	2303413	59.66%	6.784%
16	11.292	1560	1564	1569	rVB	37105	49564	1.28%	0.146%
17	11.398	1576	1582	1584	rBV	1051803	1457080	37.74%	4.291%
18	11.421	1584	1586	1590	rVV	671962	704681	18.25%	2.075%
19	11.469	1590	1594	1599	rVB	140900	193588	5.01%	0.570%
20	11.627	1615	1621	1628	rBV2	68699	109360	2.83%	0.322%
21	11.921	1662	1671	1677	rBV2	299412	581723	15.07%	1.713%
22	12.010	1682	1686	1695	rVB2	129208	257481	6.67%	0.758%
23	12.192	1713	1717	1720	rBV	48022	63556	1.65%	0.187%
24	12.221	1720	1722	1727	rVB	44073	48494	1.26%	0.143%
25	12.445	1756	1760	1763	rBV	40198	57007	1.48%	0.168%
26	12.486	1763	1767	1772	rVV5	26951	55546	1.44%	0.164%
27	12.533	1772	1775	1780	rVB	40424	56903	1.47%	0.168%
28	12.610	1783	1788	1793	rBV	824810	1031460	26.72%	3.038%
29	12.763	1807	1814	1817	rVB3	21590	39226	1.02%	0.116%
30	12.839	1820	1827	1832	rVV	652272	990595	25.66%	2.917%
31	12.886	1832	1835	1841	rVB2	42358	67210	1.74%	0.198%
32	12.980	1843	1851	1859	rBV	2406325	3229073	83.64%	9.510%
33	13.057	1859	1864	1869	rBV2	51621	95773	2.48%	0.282%
34	13.168	1875	1883	1887	rVB2	84256	164352	4.26%	0.484%
35	13.233	1890	1894	1897	rVV	41400	53011	1.37%	0.156%
36	13.274	1897	1901	1908	rVB3	62185	110462	2.86%	0.325%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.368	1913	1917	1919	rVV	31008	42667	1.11%	0.126%
38	13.398	1919	1922	1930	rVB4	34175	58632	1.52%	0.173%
39	13.680	1963	1970	1975	rBV	50819	82269	2.13%	0.242%
40	13.792	1984	1989	1992	rBV2	54086	85555	2.22%	0.252%
41	13.892	2003	2006	2012	rVB	59307	85470	2.21%	0.252%
42	14.051	2024	2033	2045	rVV2	798908	1685728	43.66%	4.965%
43	14.451	2097	2101	2105	rBV	43646	54966	1.42%	0.162%
44	14.833	2162	2166	2173	rVB2	44028	85240	2.21%	0.251%
45	15.127	2210	2216	2224	rBV	240588	569136	14.74%	1.676%
46	15.233	2231	2234	2238	rVB	32363	38998	1.01%	0.115%
47	15.433	2263	2268	2274	rVB	117184	181377	4.70%	0.534%
48	15.498	2274	2279	2284	rVB	179245	267646	6.93%	0.788%
49	15.562	2284	2290	2303	rBV	493518	850550	22.03%	2.505%
50	17.062	2539	2545	2554	rVB2	79440	181428	4.70%	0.534%
51	17.515	2615	2622	2636	rVB	55972	143178	3.71%	0.422%

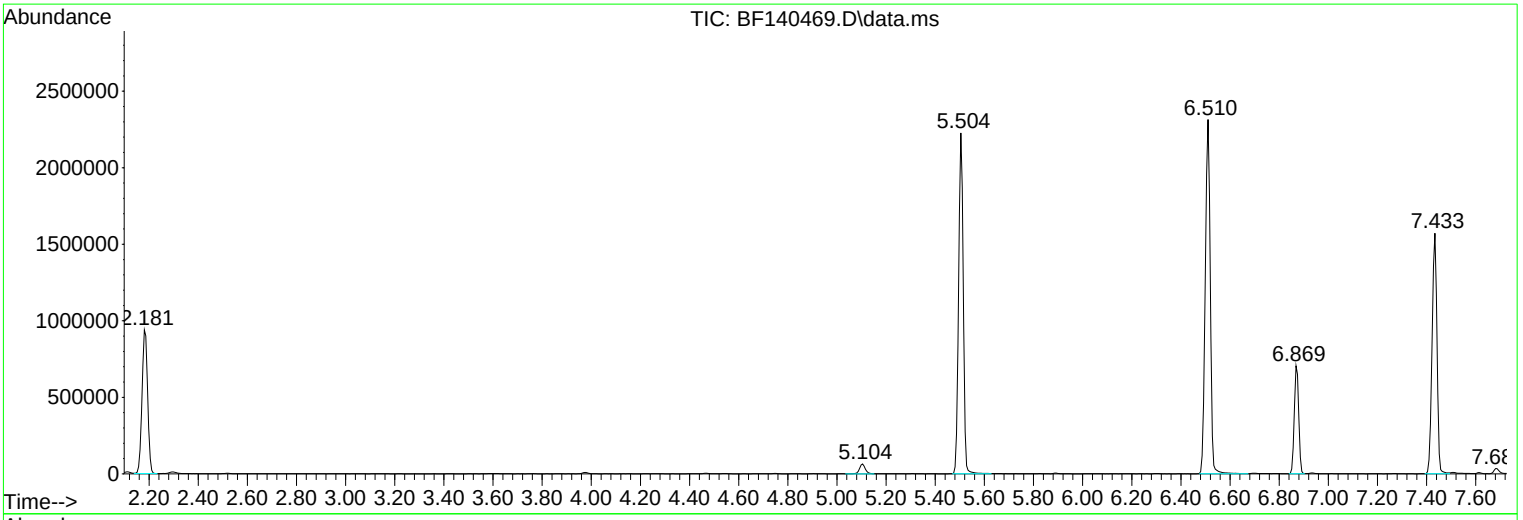
Sum of corrected areas: 33954190

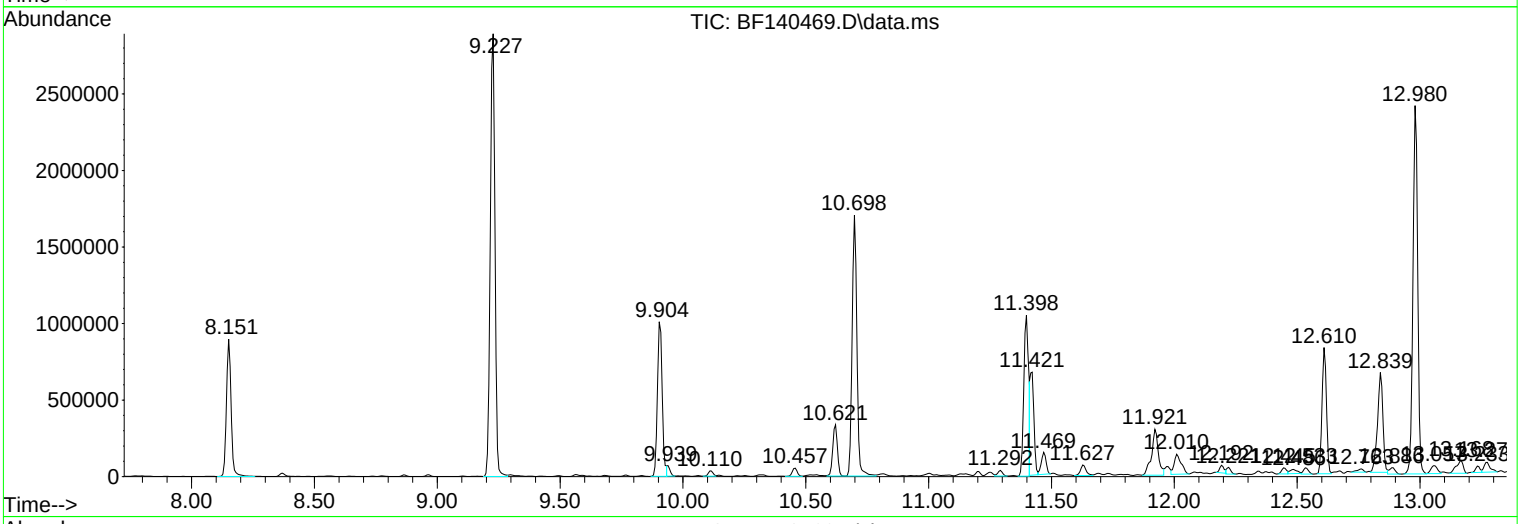
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

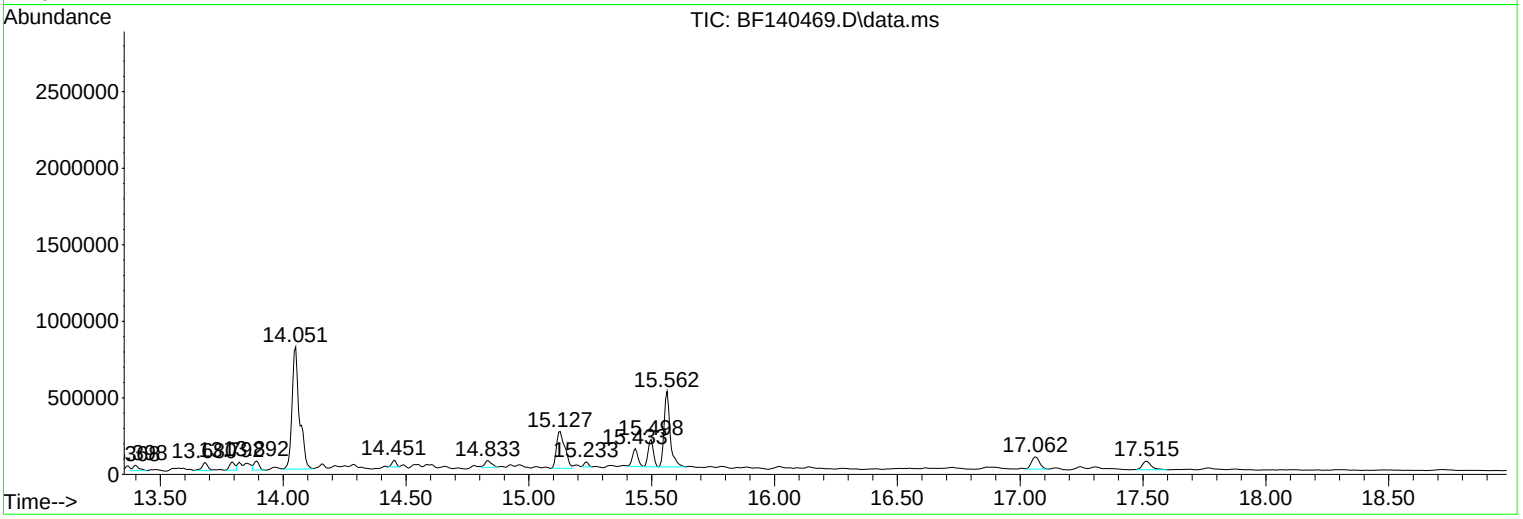
Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

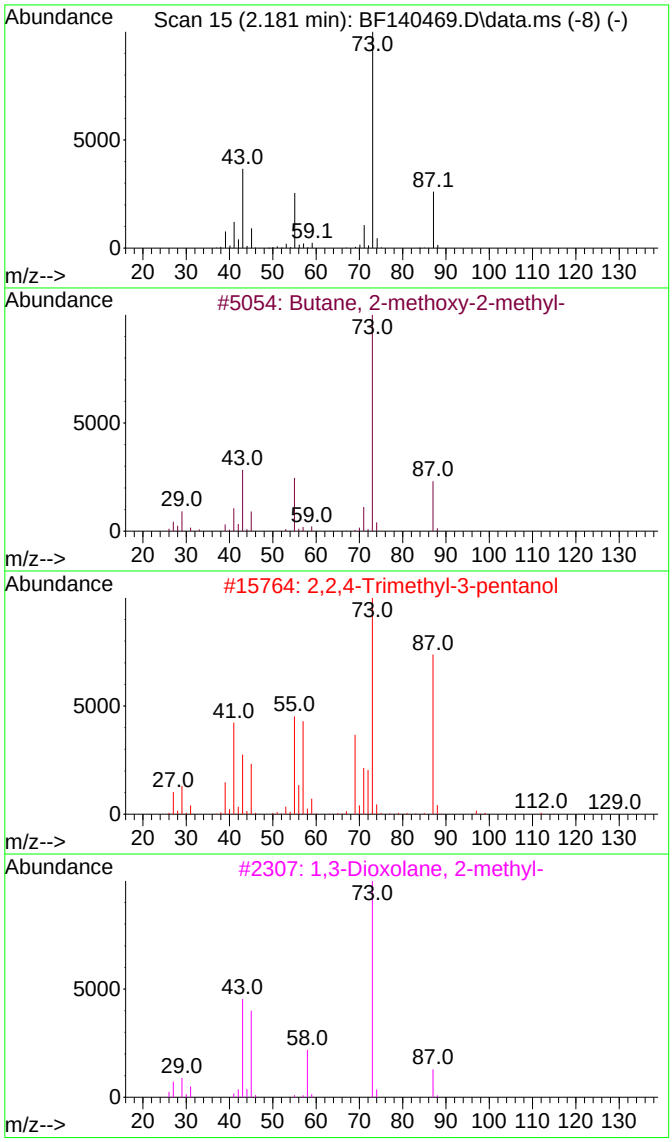
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

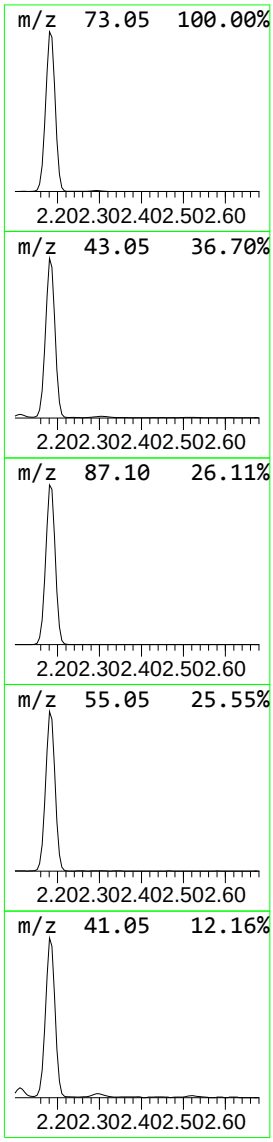
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	33.59 ng	1477190	1,4-Dichlorobenzene-d4	6.869

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

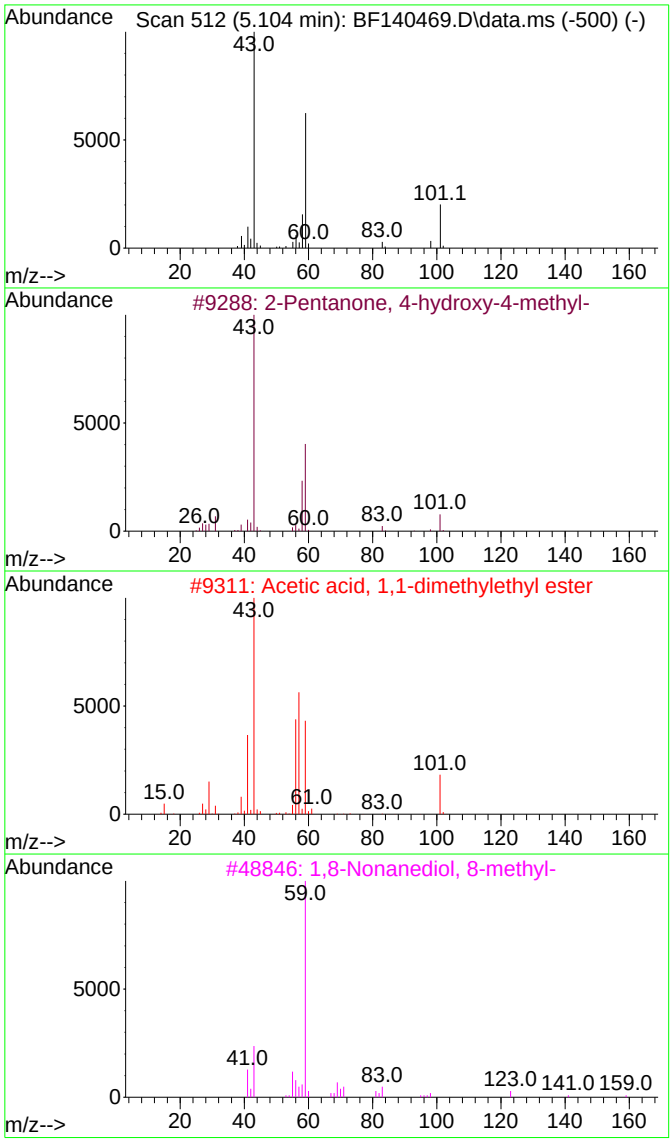
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

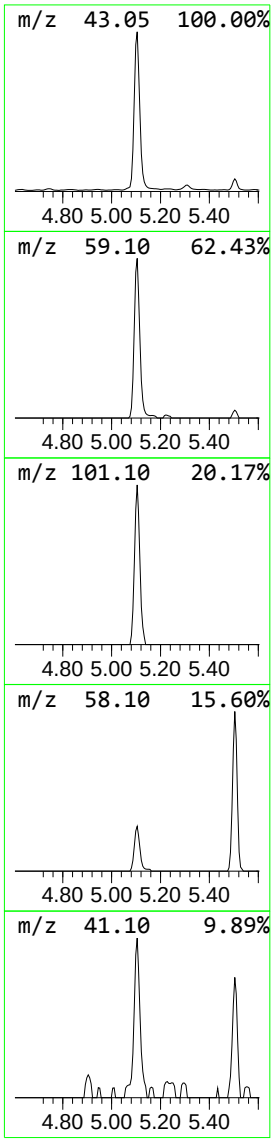
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	2.37 ng	104127	1,4-Dichlorobenzene-d4	6.869

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

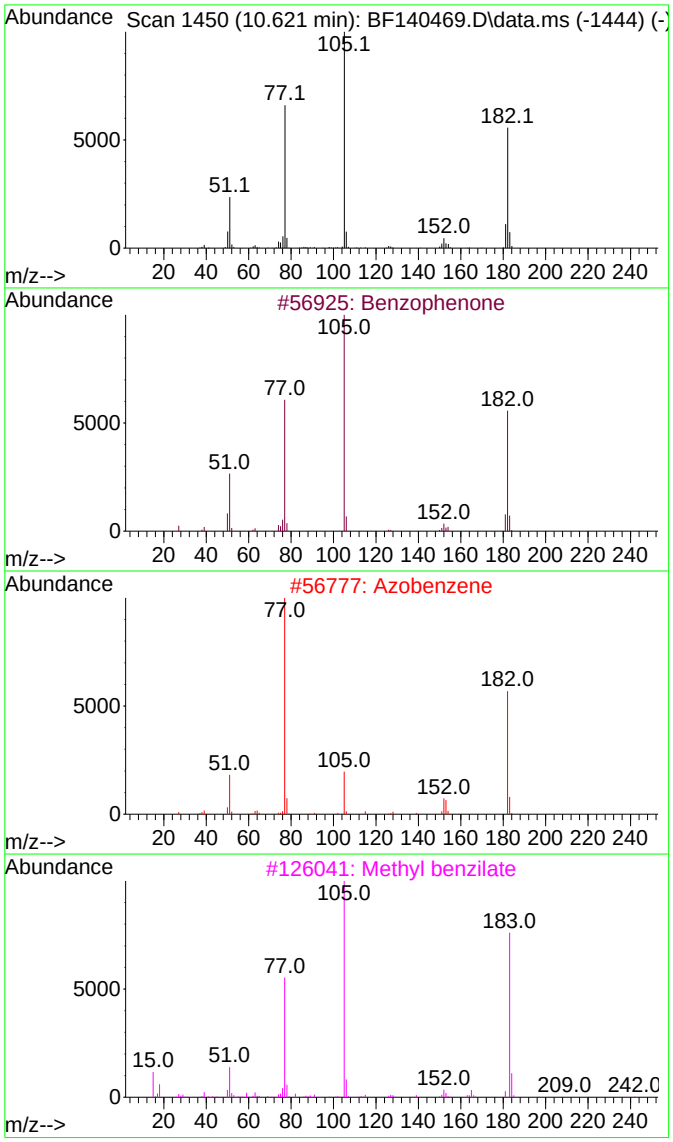
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

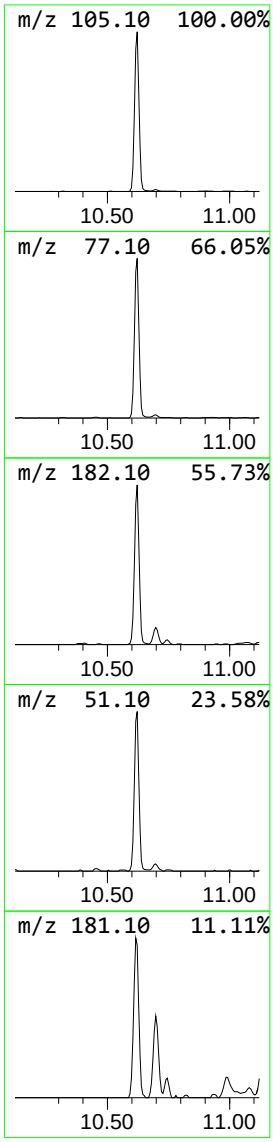
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	6.52 ng	438701	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Methyl benzilate	242	C15H14O3	000076-89-1	47
4	2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47
5	N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

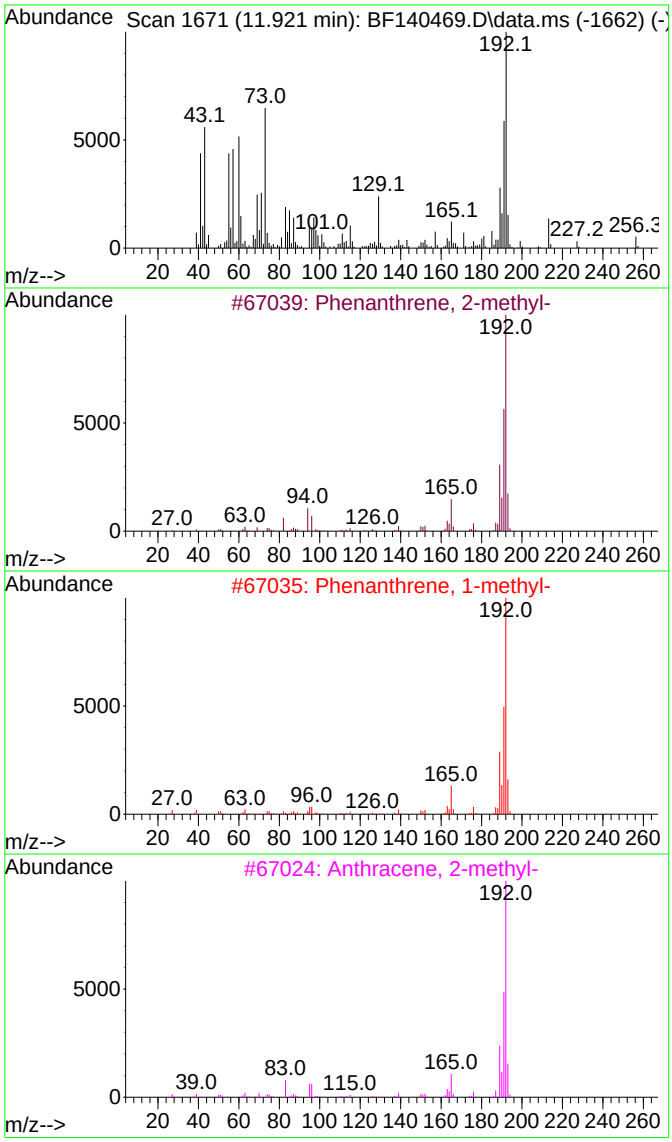
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

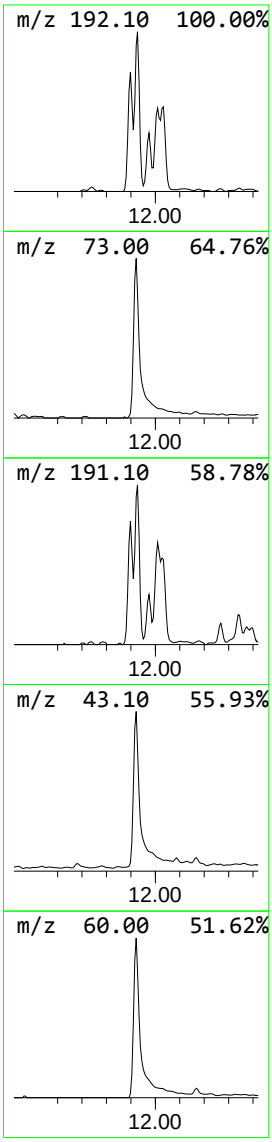
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	7.98 ng	581723	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

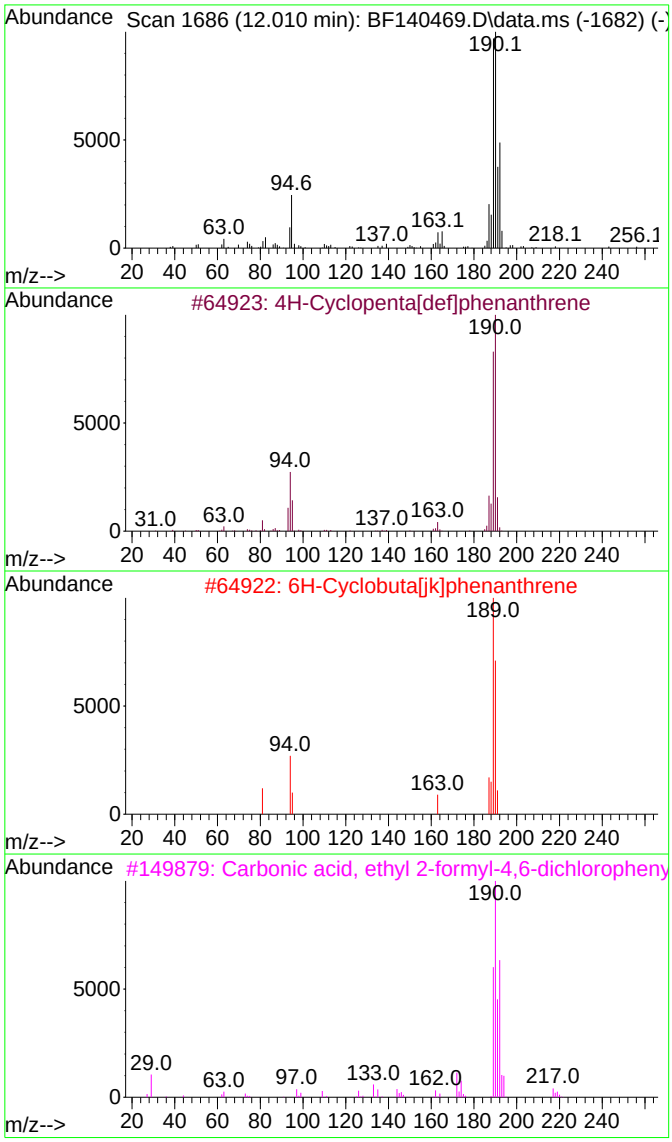
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

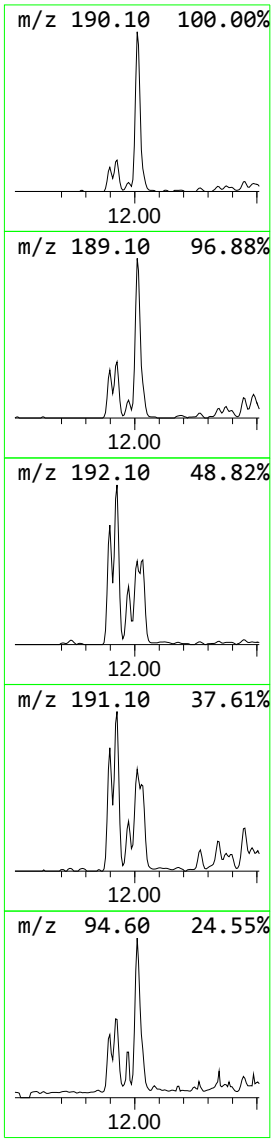
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	3.53 ng	257481	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

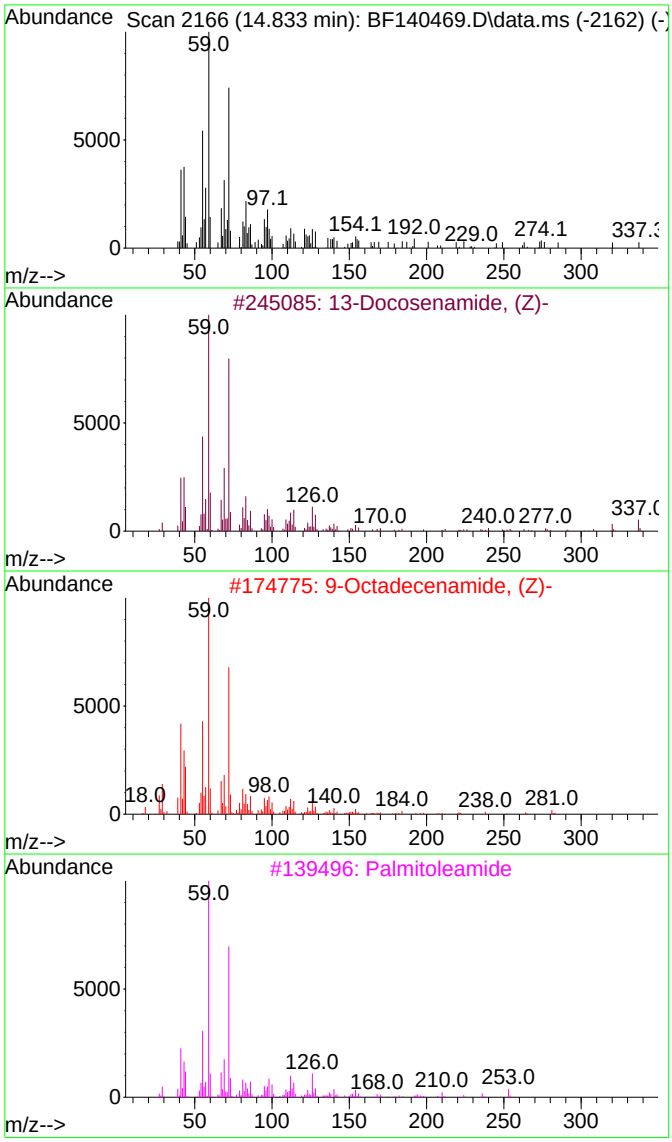
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

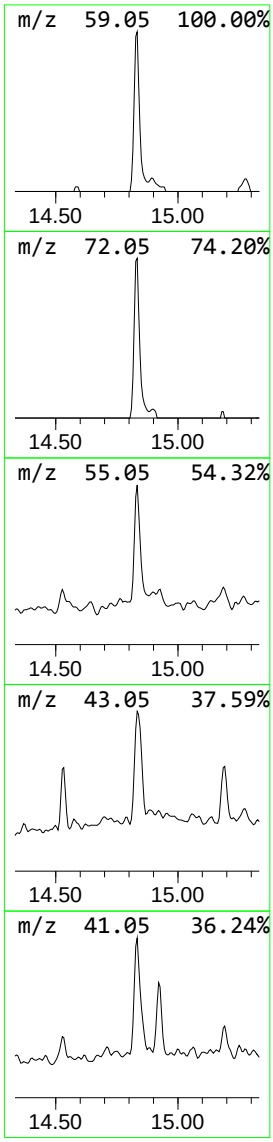
****

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.00 ng	85240	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	58
5	9-Octadecenamide	281	C18H35NO	003322-62-1	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

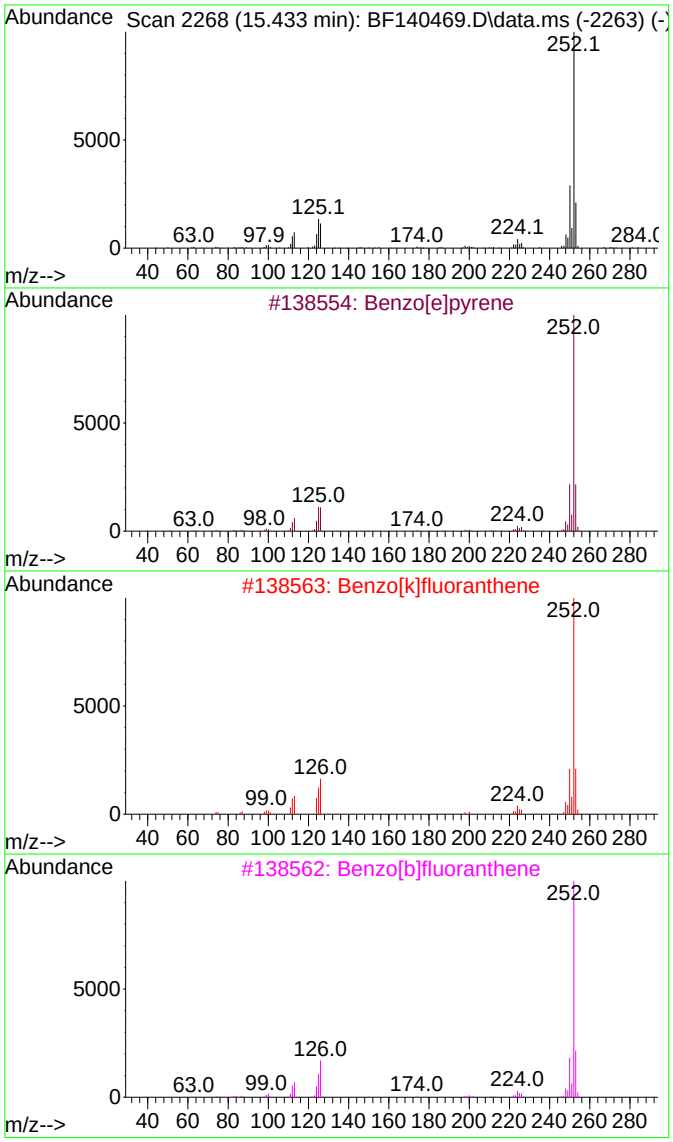
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

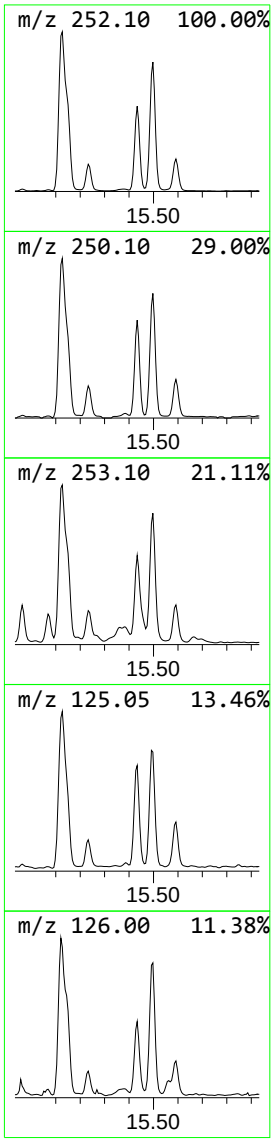
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	4.26 ng	181377	Perylene-d12	15.562

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	94
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111924\
Data File : BF140469.D
Acq On : 19 Nov 2024 13:21
Operator : RC/JU
Sample : P4852-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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...	2.181	33.6	ng	1477190	1	6.869	879593	20.0
2-Pentanone, 4-...	5.104	2.4	ng	104127	1	6.869	879593	20.0
Benzophenone	10.621	6.5	ng	438701	3	9.904	1345290	20.0
Phenanthrene, 2...	11.921	8.0	ng	581723	4	11.398	1457080	20.0
4H-Cyclopenta[d...	12.010	3.5	ng	257481	4	11.398	1457080	20.0
13-Docosenamide...	14.833	2.0	ng	85240	6	15.562	850550	20.0
Benzo[e]pyrene	15.433	4.3	ng	181377	6	15.562	850550	20.0