LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WB-303-TOP

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	18	26	rVB	1641864	2687905	89.07%	9.485%
2	3.998	317	324	331	rBV	63435	98658	3.27%	0.348%
3	5.116	505	514	521	rVB	133707	201982	6.69%	0.713%
4	5.504	573	580	585	rBV	2047239	2749407	91.10%	9.702%
5	6.504	743	750	763	rBV	1946388	2849995	94.44%	10.057%
6	6.886	810	815	820	rVB	708953	864159	28.63%	3.050%
7	7.275	876	881	887	rBV	25157	36236	1.20%	0.128%
8	7.445	902	910	915	rBV	1328779	1775839	58.84%	6.267%
9	7.698	949	953	959	rVB	67990	82701	2.74%	0.292%
10	8.169	1027	1033	1040	rBV	924185	1211624	40.15%	4.276%
11	8.380	1063	1069	1075	rVB2	24745	34967	1.16%	0.123%
12	9.245	1209	1216	1226	rBV	2234736	3017894	100.00%	10.650%
13	9.322	1226	1229	1237	rVB4	18812	34858	1.16%	0.123%
14	9.580	1265	1273	1279	rBV2	26199	49879	1.65%	0.176%
15	9.698	1290	1293	1302	rVB	22561	41847	1.39%	0.148%
16	9.780	1303	1307	1312	rBV	37162	53721	1.78%	0.190%
17	9.922	1325	1331	1335	rBV	1018088	1319688	43.73%	4.657%
18	9.957	1335	1337	1345	rVB	65713	83081	2.75%	0.293%
19	10.122	1361	1365	1369	rBV2	30246	40280	1.33%	0.142%
20	10.163	1369	1372	1377	rVB	24922	31095	1.03%	0.110%
21	10.239	1380	1385	1387	rBV2	34979	52420	1.74%	0.185%
22	10.327	1396	1400	1406	rVB3	32942	62378	2.07%	0.220%
23	10.522	1429	1433	1437	rBV3	20444	38199	1.27%	0.135%
24	10.580	1440	1443	1446	rVV2	29406	41511	1.38%	0.146%
25	10.633	1448	1452	1459	rVB	211518	274371	9.09%	0.968%
26	10.710	1459	1465	1476	rBV	1423896	1882862	62.39%	6.644%
27	10.833	1482	1486	1493	rVB3	41108	66408	2.20%	0.234%
28	11.016	1513	1517	1520	rBV2	28807	40281	1.33%	0.142%
29	11.169	1535	1543	1547	rBV6	17786	44693	1.48%	0.158%
30	11.304	1563	1566	1572	rVB3	29949	45745	1.52%	0.161%
31	11.410	1579	1584	1592	rBV	975380	1357323	44.98%	4.790%
32	11.480	1592	1596	1600	rVB2	74555	100446	3.33%	0.354%
33	11.933	1665	1673	1678	rBV2	196125	395396	13.10%	1.395%
34	11.986	1679	1682	1684	rVV2	57268	78465	2.60%	0.277%
35	12.021	1684	1688	1697	rVB	136566	286626	9.50%	1.011%
36	12.357	1739	1745	1748	rBV2	44931	77532	2.57%	0.274%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.463	1759	1763	1766	rBV	59972	80273	2.66%	0.283%
38	12.498	1766	1769	1774	rVB2	48594	75083	2.49%	0.265%
39	12.551	1775	1778	1786	rVB4	31090	64965	2.15%	0.229%
40	12.621	1786	1790	1794	rBV	156975	205253	6.80%	0.724%
41	12.663	1794	1797	1802	rVV	134957	164897	5.46%	0.582%
42	12.715	1803	1806	1813	rVB	50459	71398	2.37%	0.252%
43	12.851	1824	1829	1835	rVB	167839	240302	7.96%	0.848%
44	12.992	1848	1853	1861	rVB	1684517	2188429	72.52%	7.723%
45	13.068	1862	1866	1872	rBV2	30171	51842	1.72%	0.183%
46	13.245	1893	1896	1899	rVB	29233	31294	1.04%	0.110%
47	13.280	1899	1902	1910	rVB2	34345	49215	1.63%	0.174%
48	13.892	2002	2006	2014	rVB	53178	98021	3.25%	0.346%
49	14.045	2026	2032	2044	rBV2	586496	926845	30.71%	3.271%
50	15.092	2205	2210	2219	rBV	53684	123912	4.11%	0.437%
51	15.398	2258	2262	2267	rVV	37932	56790	1.88%	0.200%
52	15.456	2268	2272	2278	rVV	61783	94475	3.13%	0.333%
53	15.527	2278	2284	2296	rVB	467621	782883	25.94%	2.763%
54	17.009	2532	2536	2543	rBV2	14439	32326	1.07%	0.114%
55	17.286	2576	2583	2591	rVB3	49087	110459	3.66%	0.390%
56	17.856	2674	2680	2689	rVB2	32305	82251	2.73%	0.290%
57	18.109	2718	2723	2730	rBV7	12244	34133	1.13%	0.120%
58	18.227	2733	2743	2767	rVB4	125424	460872	15.27%	1.626%
59	18.468	2774	2784	2786	rBV7	78481	201119	6.66%	0.710%

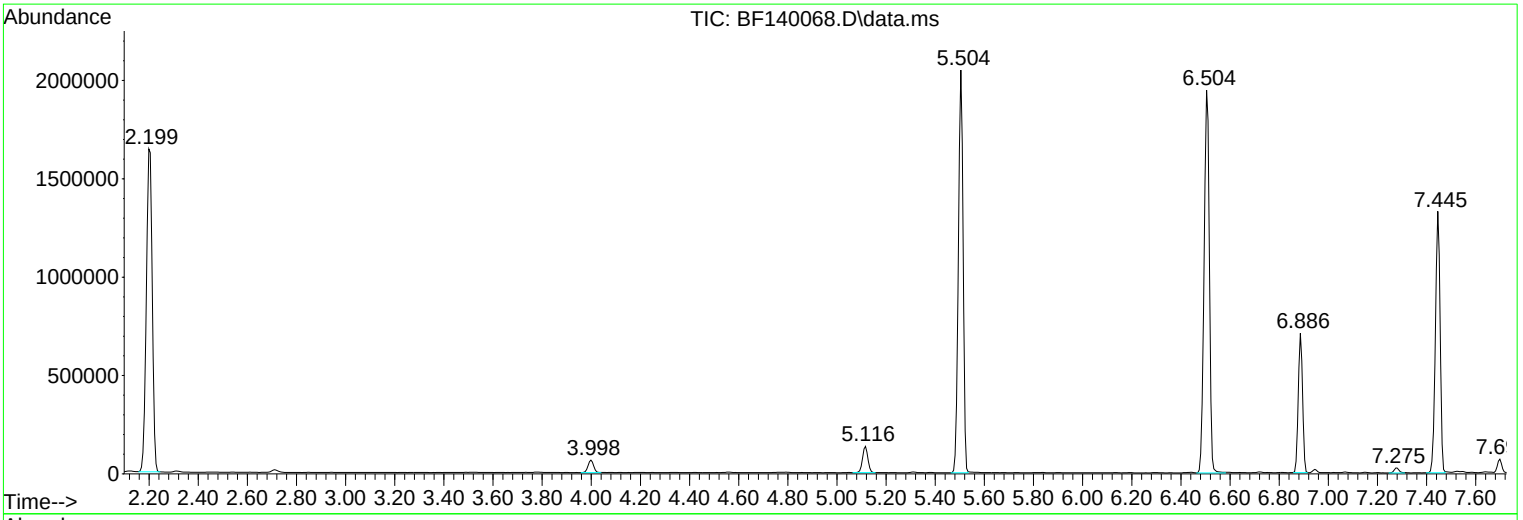
Sum of corrected areas: 28337509

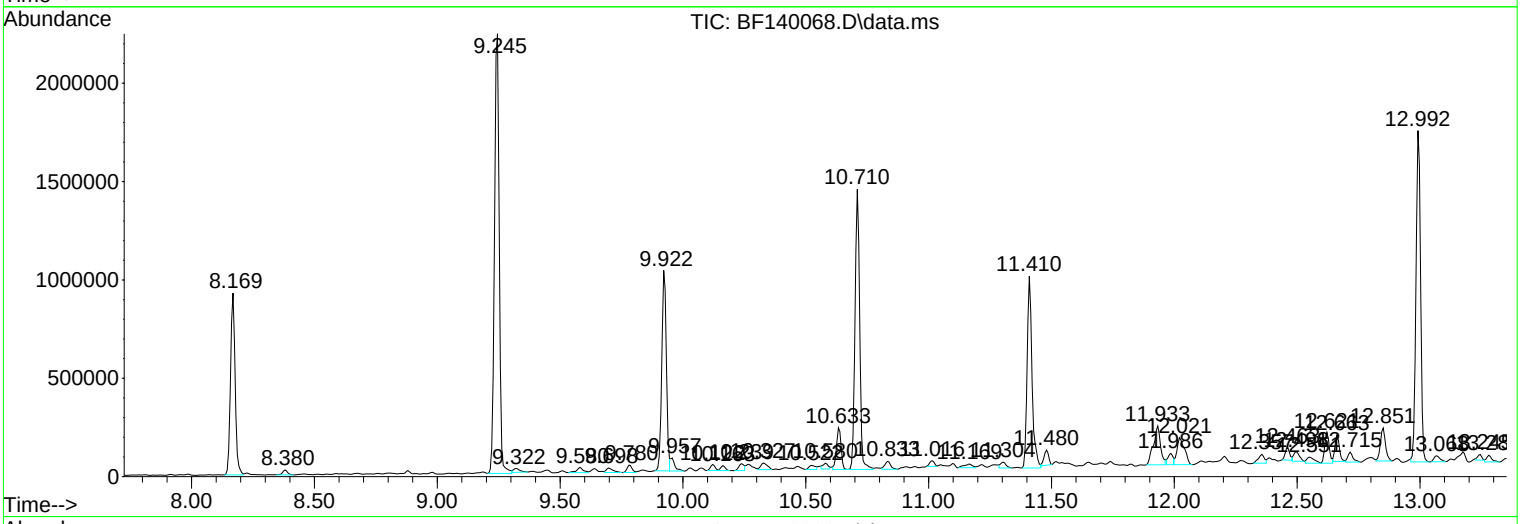
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

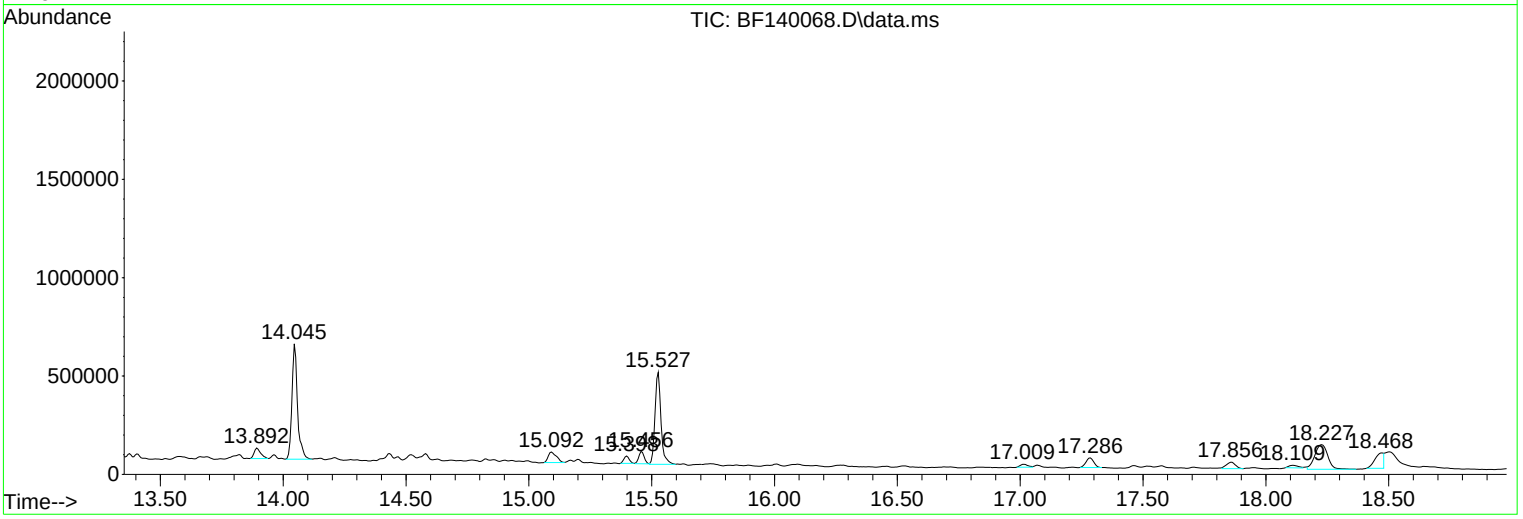
Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

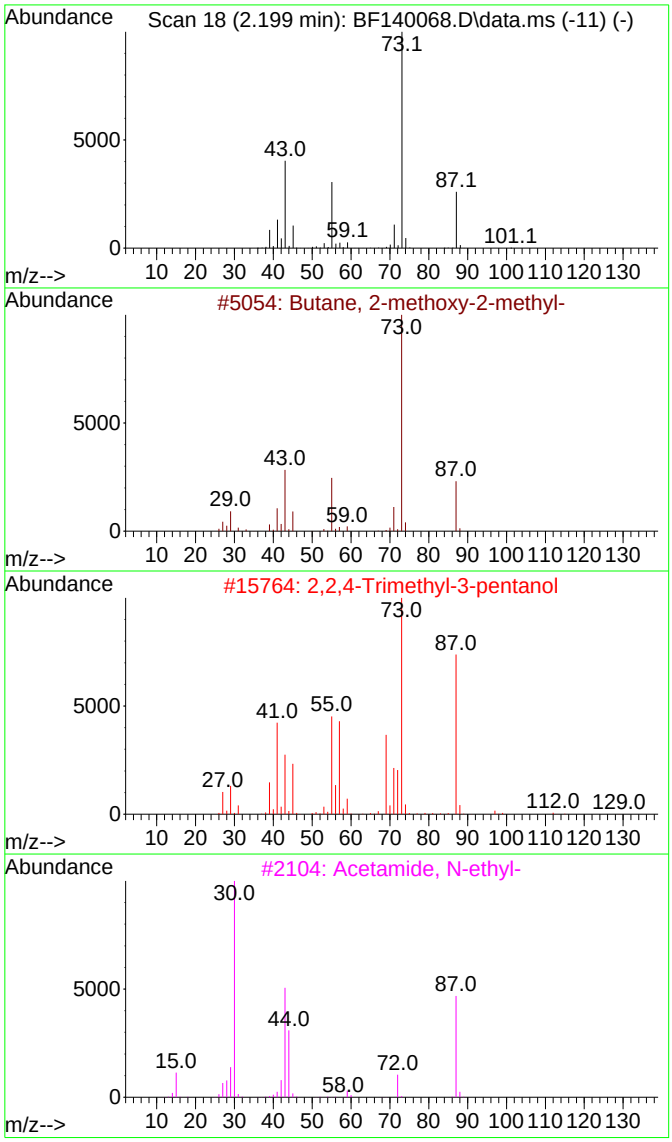
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

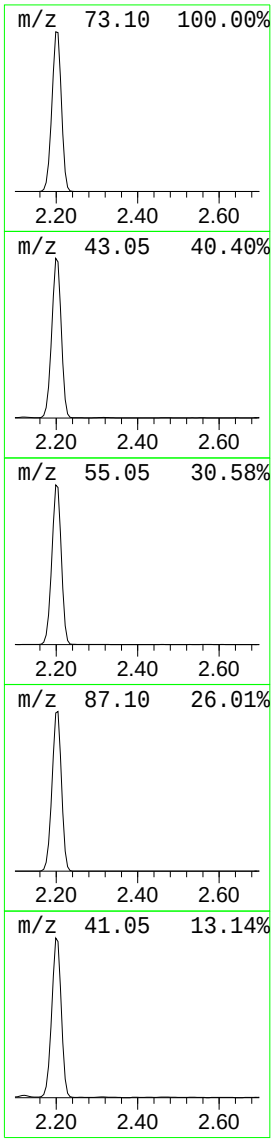
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	62.21 ng	2687910	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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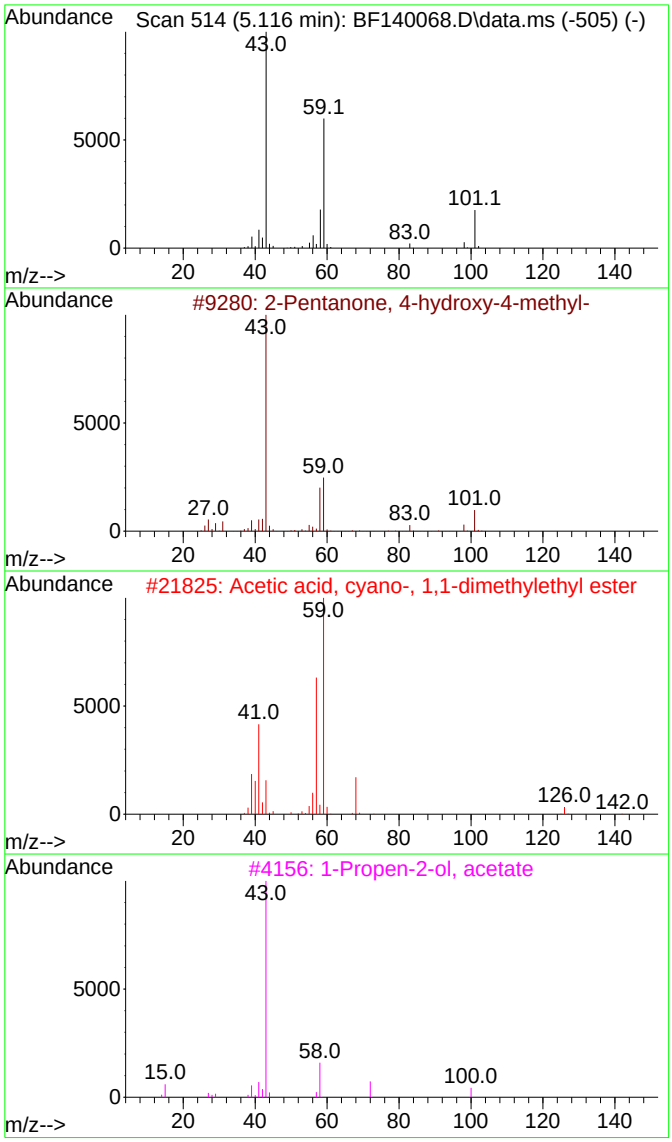
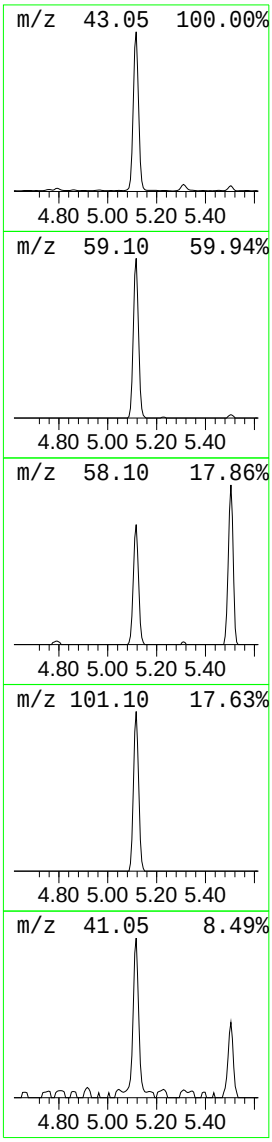
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	4.67 ng	201982	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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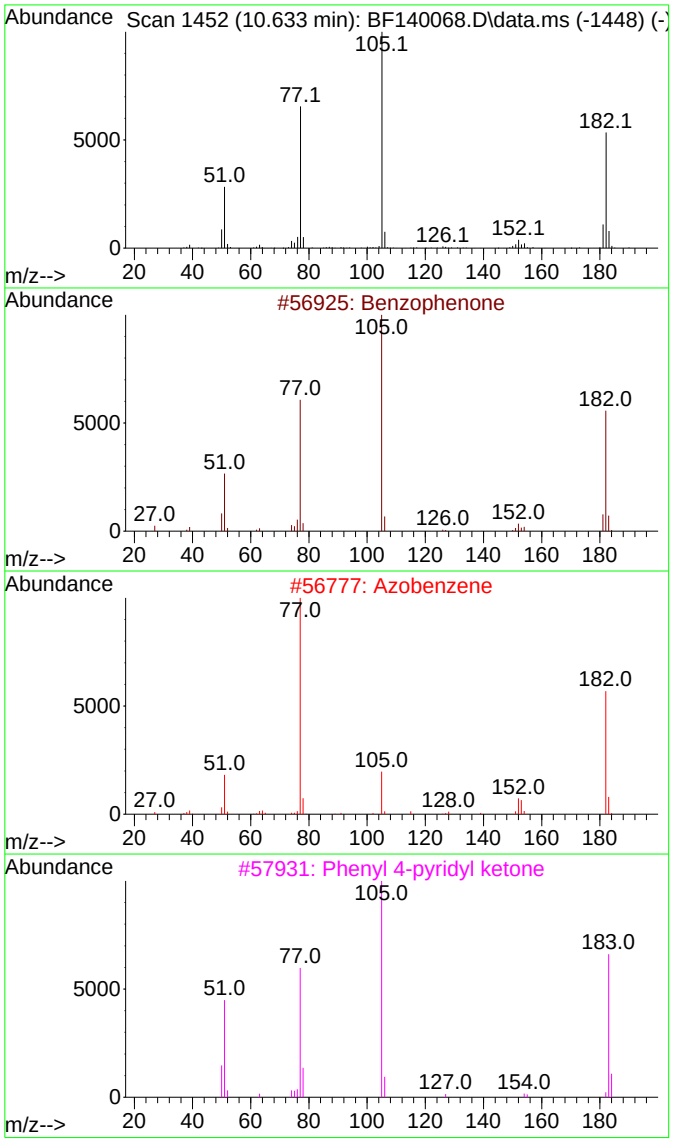
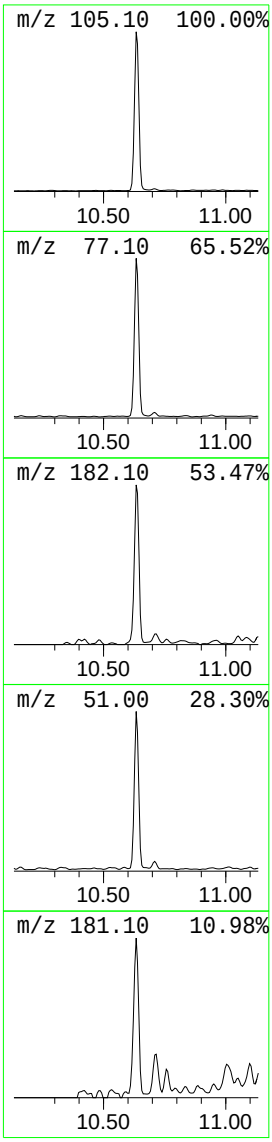
Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	4.16 ng	274371	Acenaphthene-d10	9.922

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	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4	Benzoylformic acid	150	C8H6O3	000611-73-4	49
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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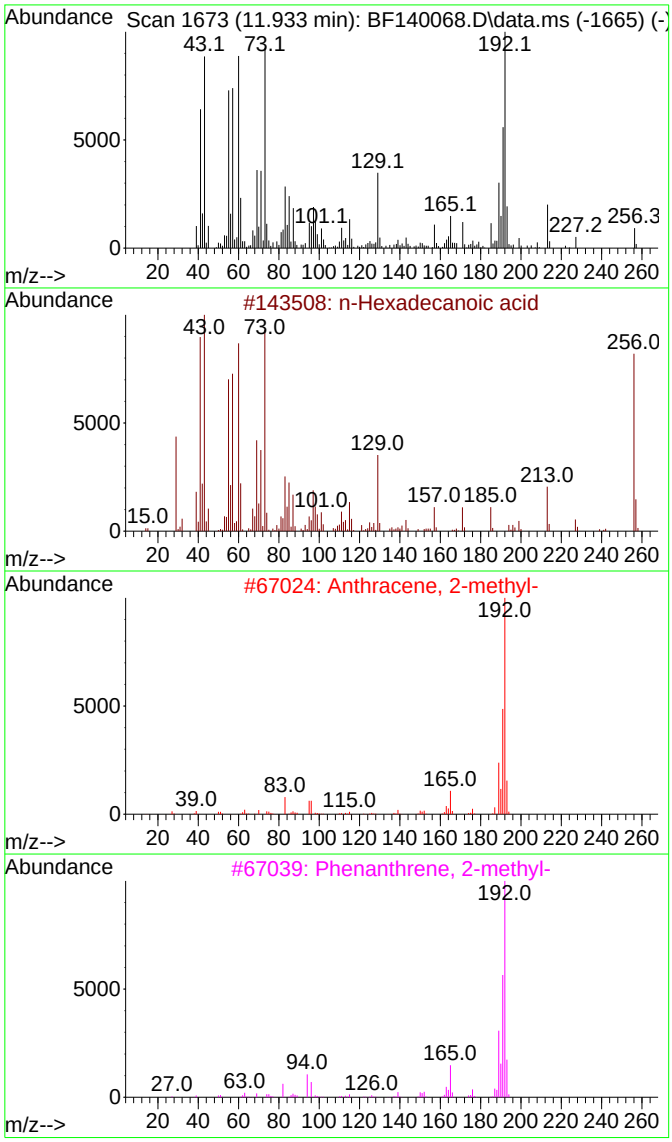
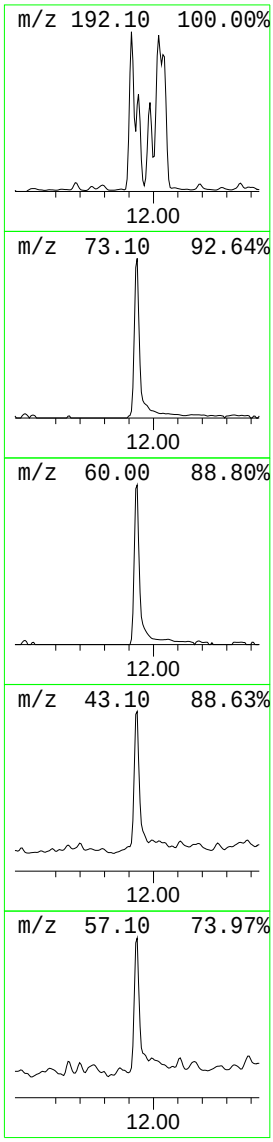
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.83 ng	395396	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	86
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

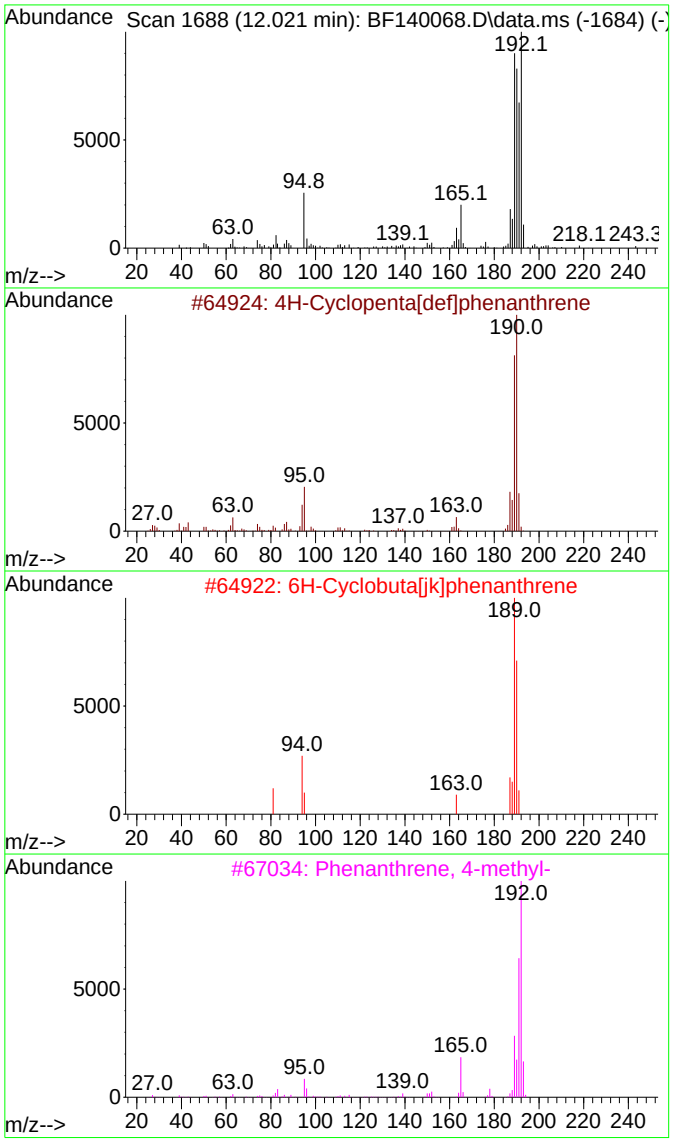
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

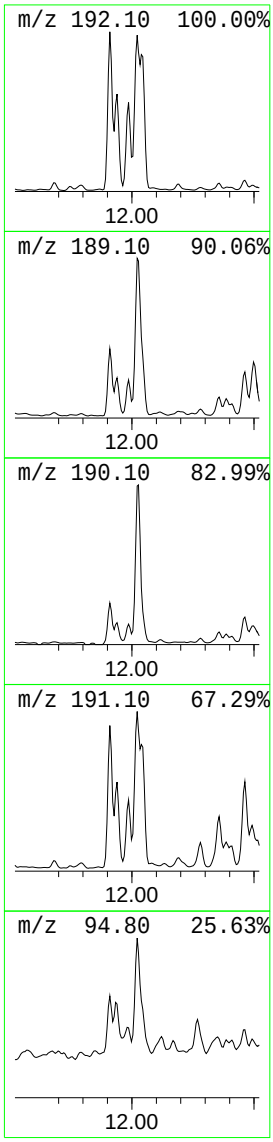
****

Peak Number 6 unknown12.021 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.021	4.22 ng	286626	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	46
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	41
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	41





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Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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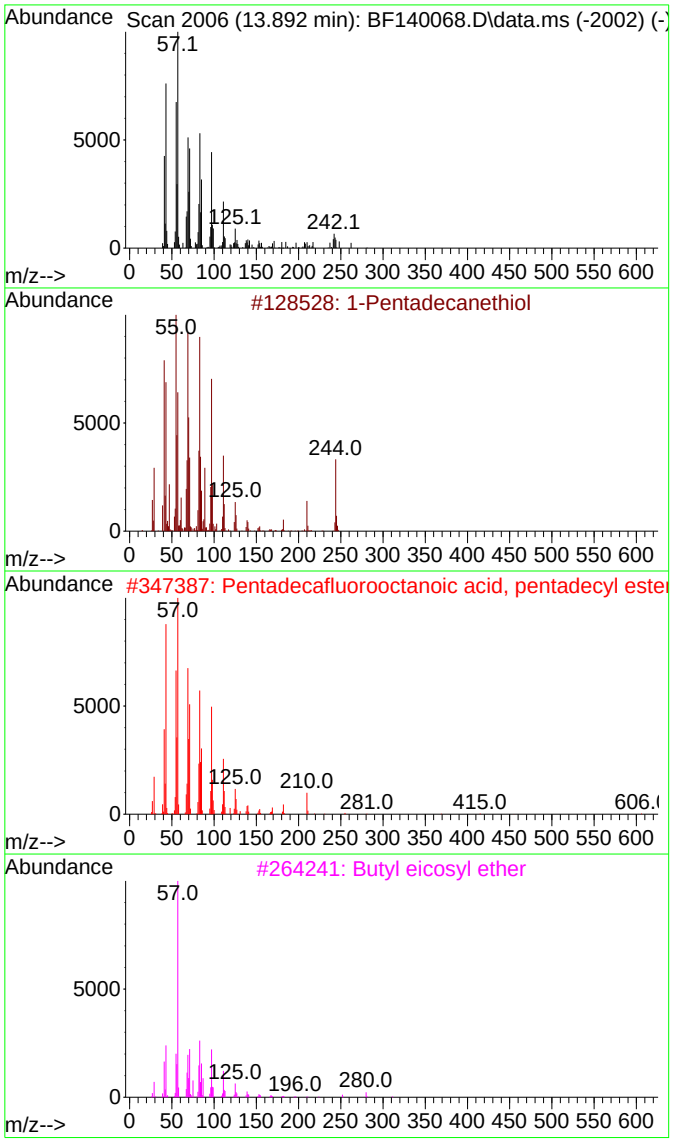
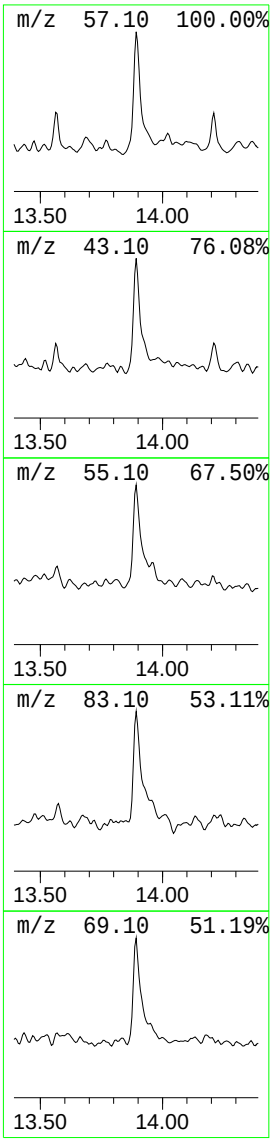
Peak Number 7 1-Pentadecanethiol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.12 ng	98021	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	93
2	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91
3	Butyl eicosyl ether	354	C24H50O	1000406-40-7	91
4	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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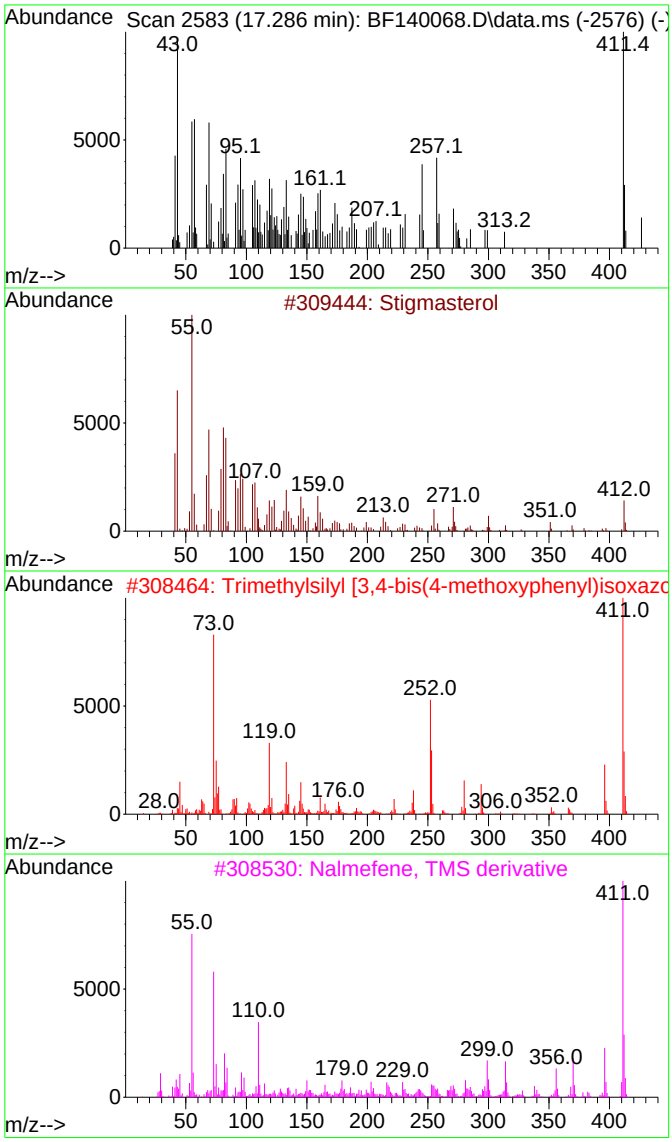
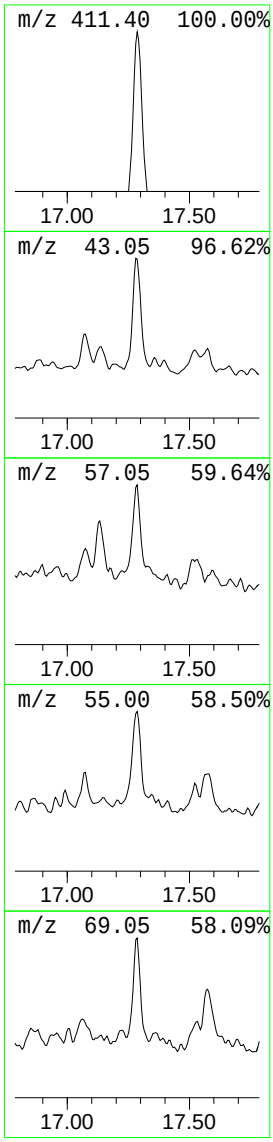
Peak Number 8 unknown17.286 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	2.82 ng	110459	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	46
2	Trimethylsilyl [3,4-bis(4-methox...	411	C22H25NO5Si	1000476-35-5	25
3	Nalmefene, TMS derivative	411	C24H33NO3Si	1000333-47-8	22
4	Silane, methylvinyl(hept-4-yloxy...	454	C28H58O2Si	1000416-98-6	22
5	Silane, methylvinyl(2,4-dimethyl...	454	C28H58O2Si	1010416-92-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

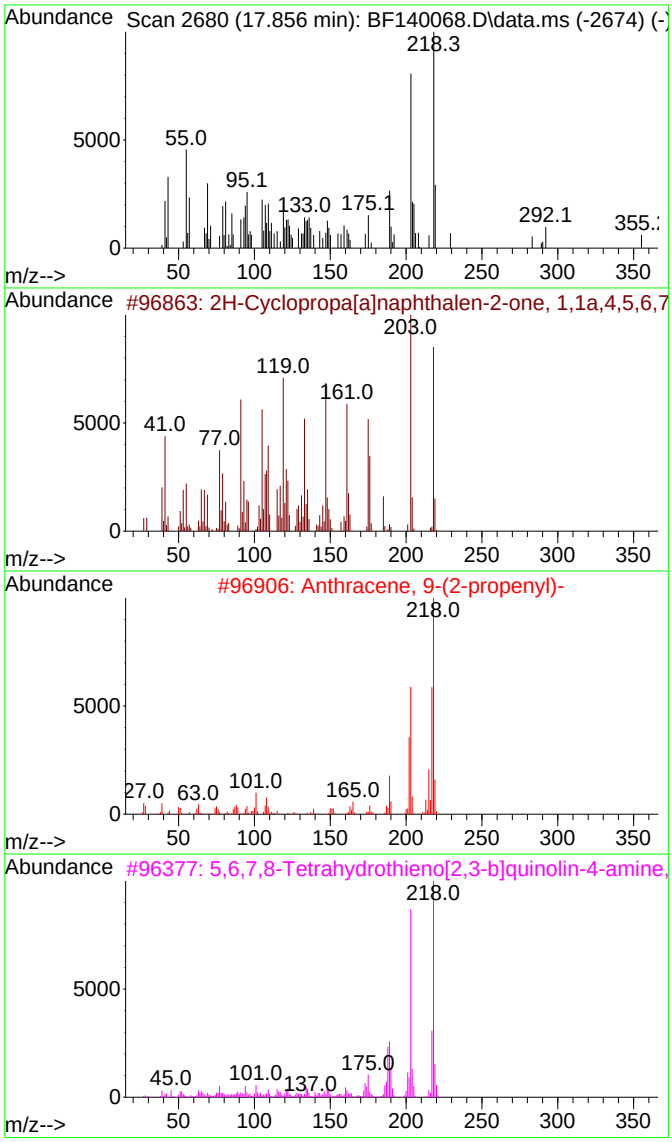
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

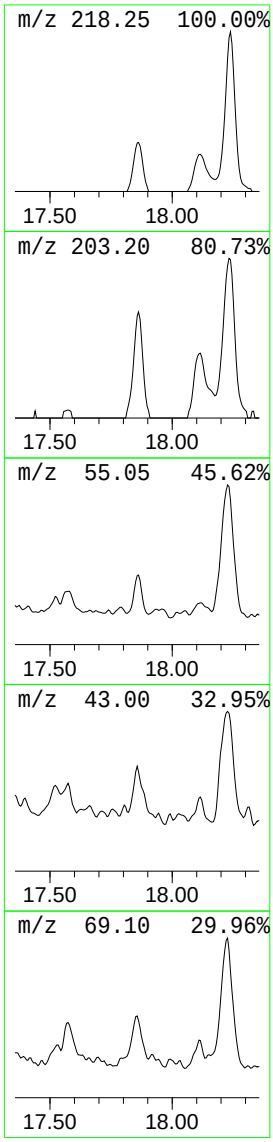
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2H-Cyclopropa[a]naphthalen-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.856	2.10 ng	82251	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	76
2	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	52
3	5,6,7,8-Tetrahydrothieno[2,3-b]q...	218	C12H14N2S	134315-44-9	52
4	2-Chloro-5,6-dimethyl-1-(2-propy...	218	C12H11ClN2	080276-20-6	52
5	1,3-Dimethyl-4,6-bis(1-methyl-1-...	274	C16H26Si2	1000293-75-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

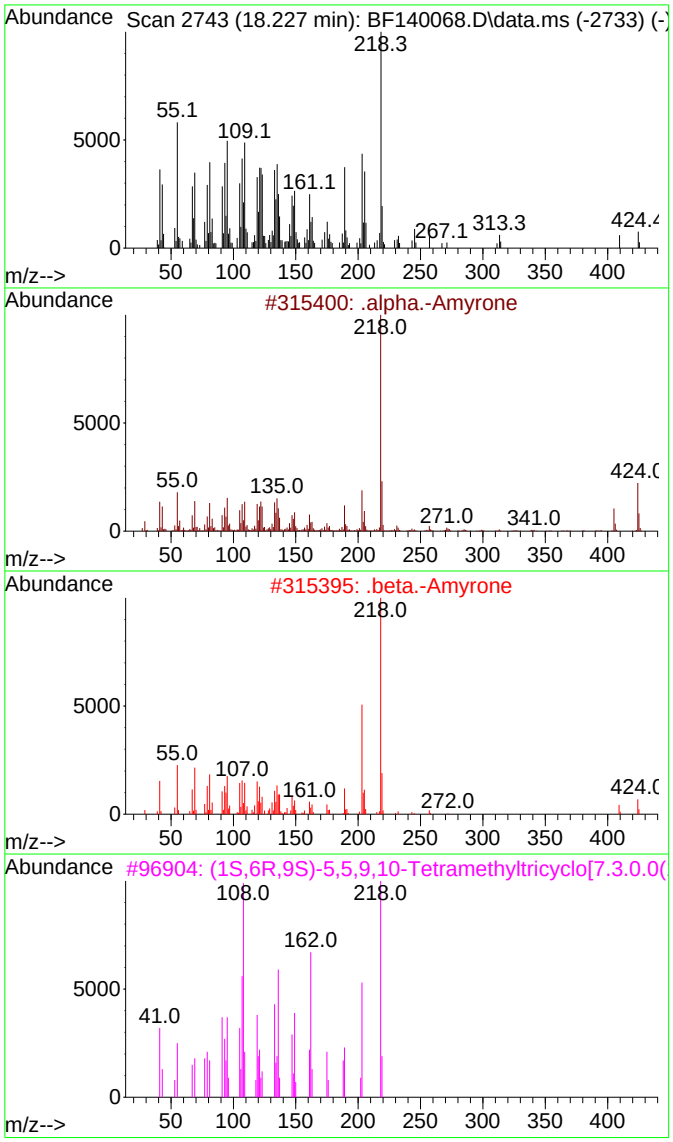
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

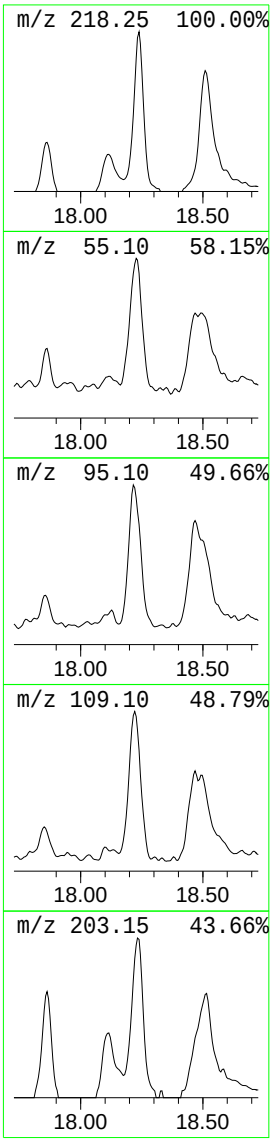
****

Peak Number 10 .alpha.-Amyrone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	11.77 ng	460872	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrone	424	C30H48O	000638-96-0	98
2	.beta.-Amyrone	424	C30H48O	000638-97-1	60
3	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	53
4	5H-3,5a-Epoxynaphth[2,1-c]oxepin...	278	C18H30O2	001153-34-0	52
5	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

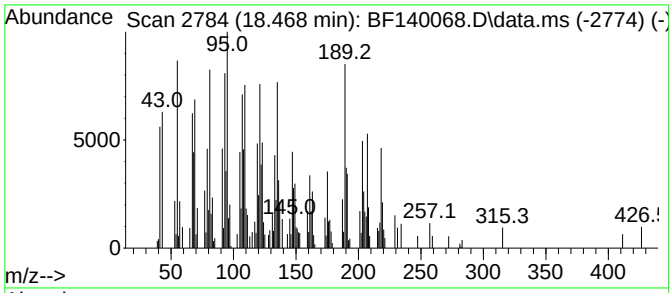
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

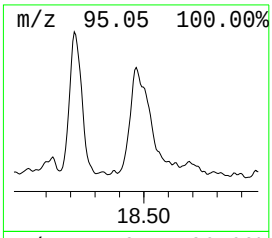
****

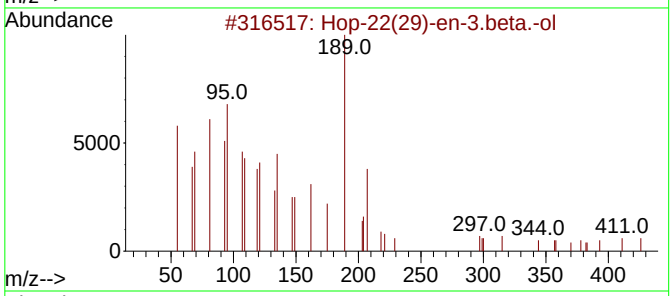
Peak Number 11 Hop-22(29)-en-3.beta.-ol Concentration Rank 4

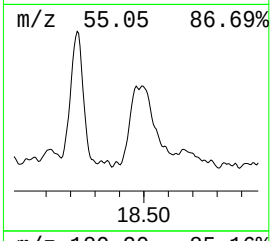
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.468	5.14 ng	201119	Perylene-d12	15.527

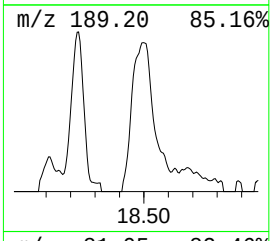
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	56
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	50
3	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	45
4	4,8-Methanoazulen-9-ol, decahydr...	222	C15H26O	004586-22-5	43
5	Thunbergol	290	C20H34O	025269-17-4	42

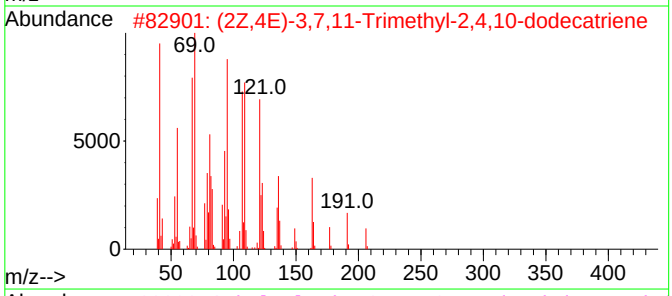


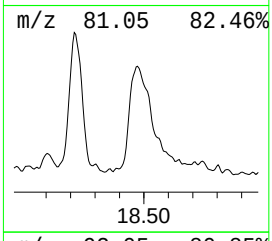


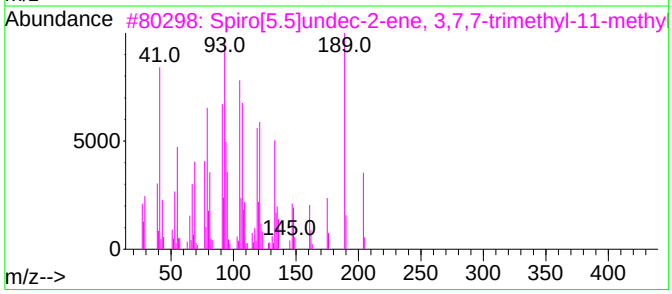


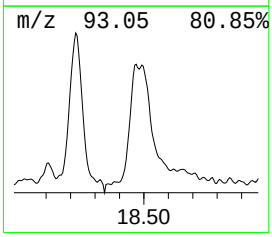












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102624\
Data File : BF140068.D
Acq On : 26 Oct 2024 19:09
Operator : RC/JU
Sample : P4460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-303-TOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.199	62.2	ng	2687910	1	6.886	864159	20.0
2-Pentanone, 4-...	5.116	4.7	ng	201982	1	6.886	864159	20.0
Benzophenone	10.633	4.2	ng	274371	3	9.922	1319690	20.0
n-Hexadecanoic ...	11.933	5.8	ng	395396	4	11.410	1357320	20.0
unknown12.021	12.021	4.2	ng	286626	4	11.410	1357320	20.0
1-Pentadecanethiol	13.892	2.1	ng	98021	5	14.045	926845	20.0
unknown17.286	17.286	2.8	ng	110459	6	15.527	782883	20.0
2H-Cyclopropa[a...	17.856	2.1	ng	82251	6	15.527	782883	20.0
.alpha.-Amyrone	18.227	11.8	ng	460872	6	15.527	782883	20.0
Hop-22(29)-en-3...	18.468	5.1	ng	201119	6	15.527	782883	20.0