LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123471.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	28	rVB	1118625	1400535	29.95%	3.681%
2	2.322	37	40	47	rVB	75126	98316	2.10%	0.258%
3	5.128	513	517	522	rVB	71574	82677	1.77%	0.217%
4	5.516	578	583	587	rBV	4443168	4461019	95.40%	11.724%
5	6.522	749	754	761	rBV	4567550	4671668	99.90%	12.278%
6	6.722	785	788	794	rBV	57675	68478	1.46%	0.180%
7	6.898	814	818	822	rBV	1701402	1323377	28.30%	3.478%
8	7.457	908	913	916	rBV	2977603	2930648	62.67%	7.702%
9	8.186	1032	1037	1040	rBV	1941355	1686747	36.07%	4.433%
10	8.869	1148	1153	1156	rBV	509416	605675	12.95%	1.592%
11	8.898	1156	1158	1163	rVB	78291	76333	1.63%	0.201%
12	9.263	1215	1220	1223	rBV	5676875	4676174	100.00%	12.290%
13	9.374	1236	1239	1243	rVB	115585	109885	2.35%	0.289%
14	9.651	1283	1286	1291	rBV	244431	218054	4.66%	0.573%
15	9.874	1319	1324	1329	rVB	52685	58232	1.25%	0.153%
16	9.945	1332	1336	1339	rVV	1960208	1683443	36.00%	4.424%
17	10.727	1465	1469	1473	rBV	2658606	2412719	51.60%	6.341%
18	11.145	1535	1540	1547	rBV	353543	340201	7.28%	0.894%
19	11.386	1578	1581	1585	rBV	88065	75332	1.61%	0.198%
20	11.433	1585	1589	1591	rVV	1590843	1398088	29.90%	3.674%
21	11.451	1591	1592	1596	rVB	182451	142413	3.05%	0.374%
22	11.645	1622	1625	1629	rBV2	100260	104058	2.23%	0.273%
23	11.827	1651	1656	1658	rBV	101279	81645	1.75%	0.215%
24	11.957	1675	1678	1682	rBV2	251434	196080	4.19%	0.515%
25	12.515	1770	1773	1775	rBV2	97041	109016	2.33%	0.287%
26	12.533	1775	1776	1779	rVB2	97617	75906	1.62%	0.199%
27	12.645	1792	1795	1798	rVB	510167	394186	8.43%	1.036%
28	12.874	1828	1834	1837	rBV	413998	421635	9.02%	1.108%
29	13.021	1855	1859	1862	rBV	3839863	3202747	68.49%	8.417%
30	13.204	1888	1890	1894	rVB	70574	63297	1.35%	0.166%
31	13.274	1897	1902	1905	rVV2	66442	81011	1.73%	0.213%
32	13.709	1974	1976	1982	rVB2	47476	58651	1.25%	0.154%
33	13.951	2012	2017	2026	rBV5	209280	414087	8.86%	1.088%
34	14.080	2033	2039	2041	rBV2	1407369	1512379	32.34%	3.975%
35	14.104	2041	2043	2046	rVB	292989	220879	4.72%	0.580%
36	14.186	2054	2057	2059	rBV	95639	82087	1.76%	0.216%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.556	2117	2120	2123	rVB2	112740	103873	2.22%	0.273%
38	14.592	2123	2126	2128	rBV3	110535	141634	3.03%	0.372%
39	15.139	2215	2219	2222	rBV	305542	479166	10.25%	1.259%
40	15.451	2268	2272	2277	rVB	201989	270645	5.79%	0.711%
41	15.509	2279	2282	2286	rVB	244067	269145	5.76%	0.707%
42	15.580	2289	2294	2297	rBV2	709761	922456	19.73%	2.424%
43	16.080	2376	2379	2385	rVB	77987	109801	2.35%	0.289%
44	17.080	2546	2549	2556	rVB3	112002	215546	4.61%	0.566%

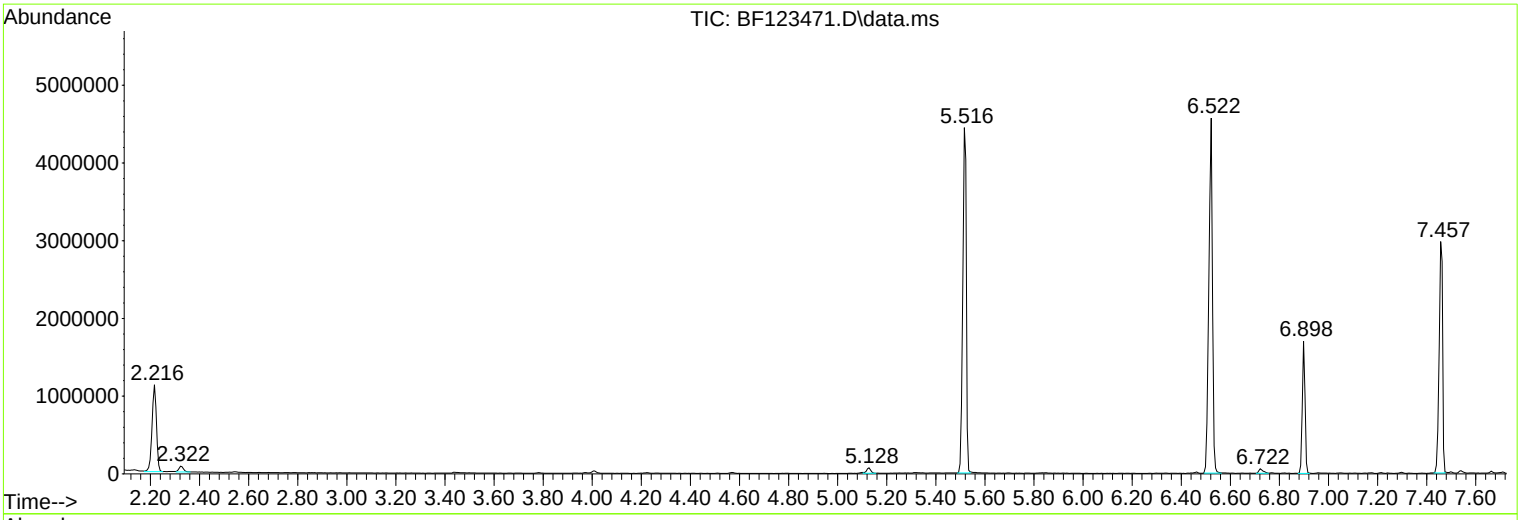
Sum of corrected areas: 38049944

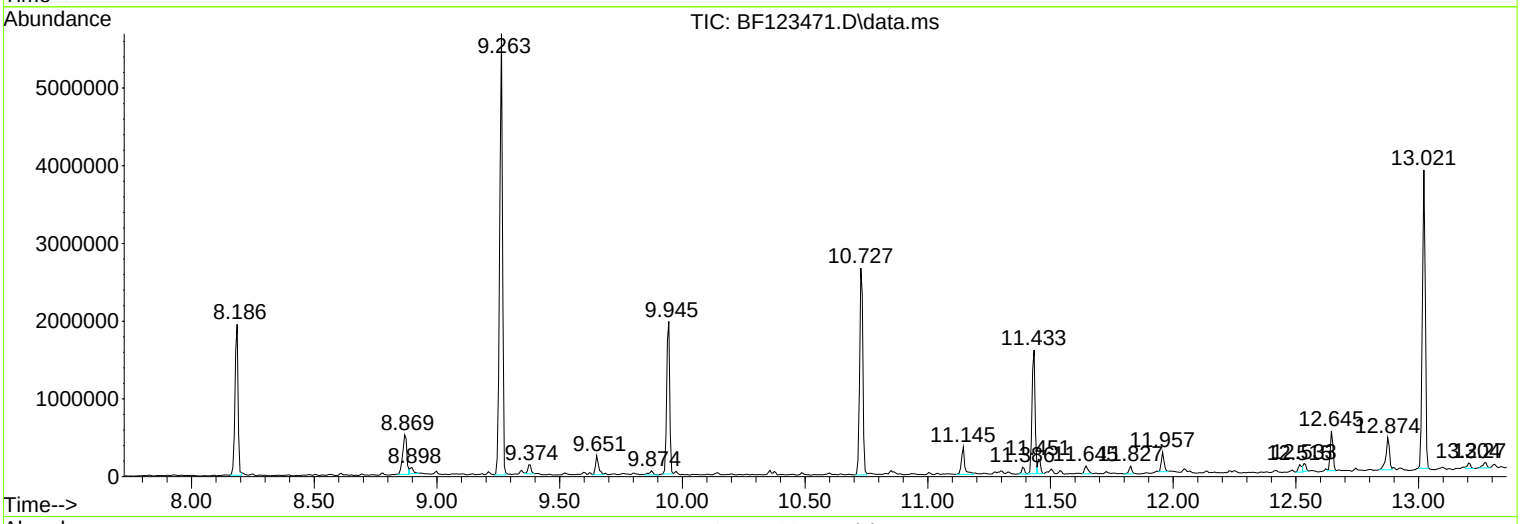
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

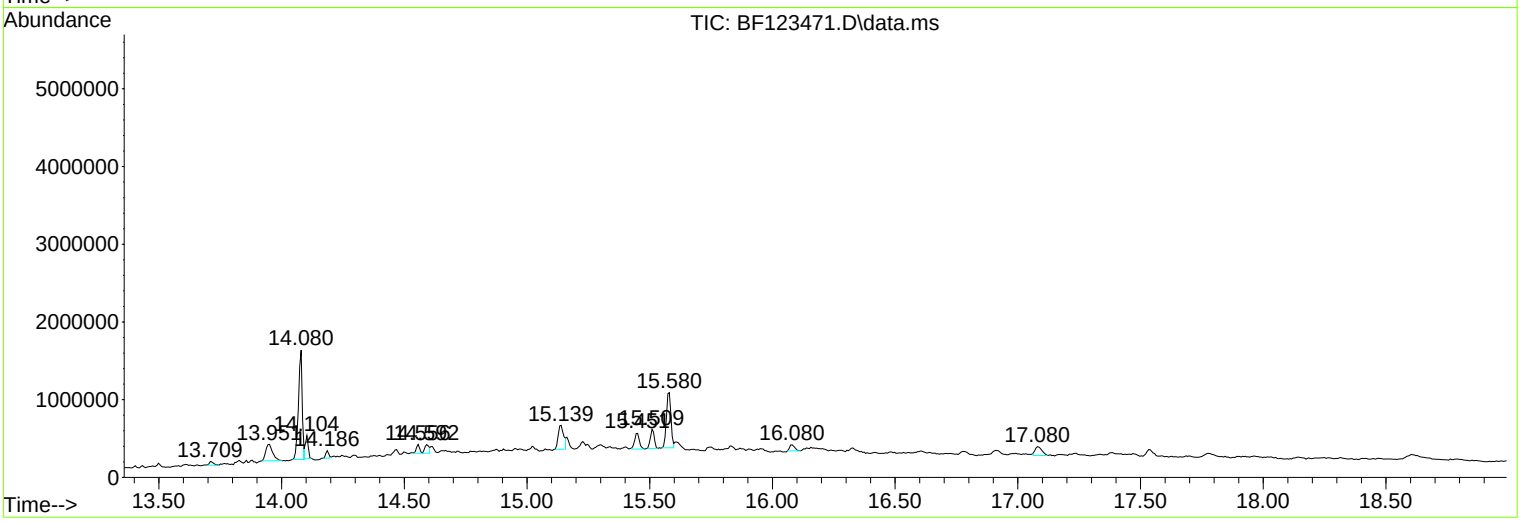
Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

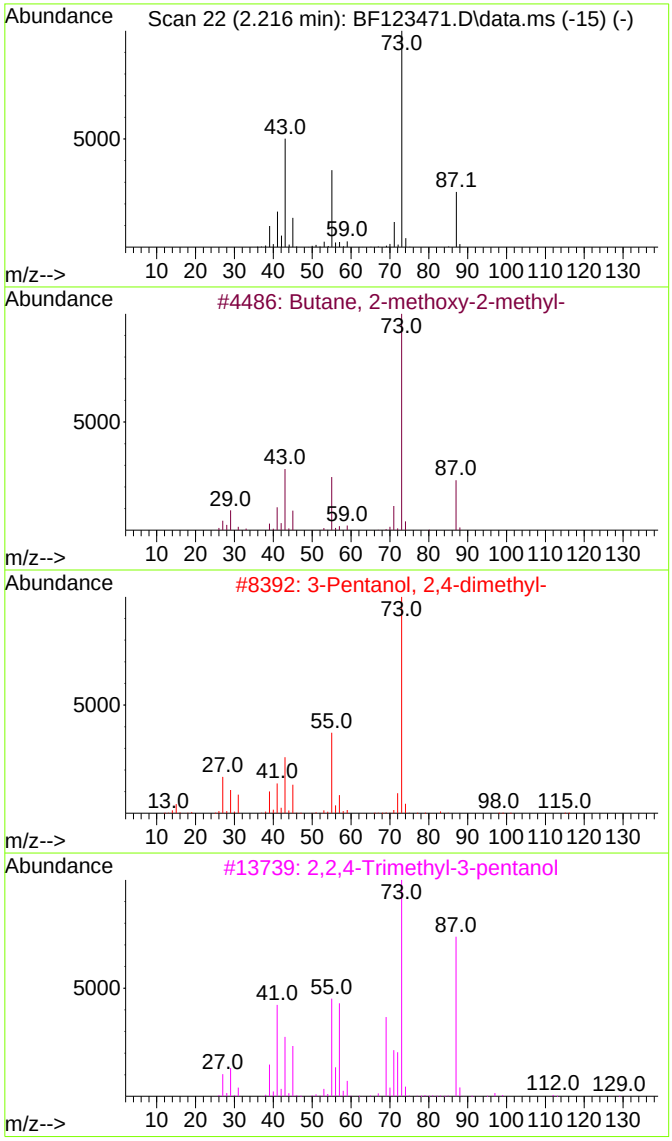
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

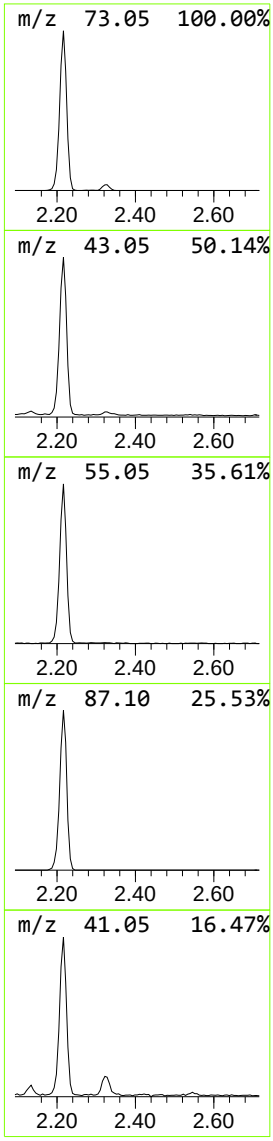
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	21.17 ng	1400540	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

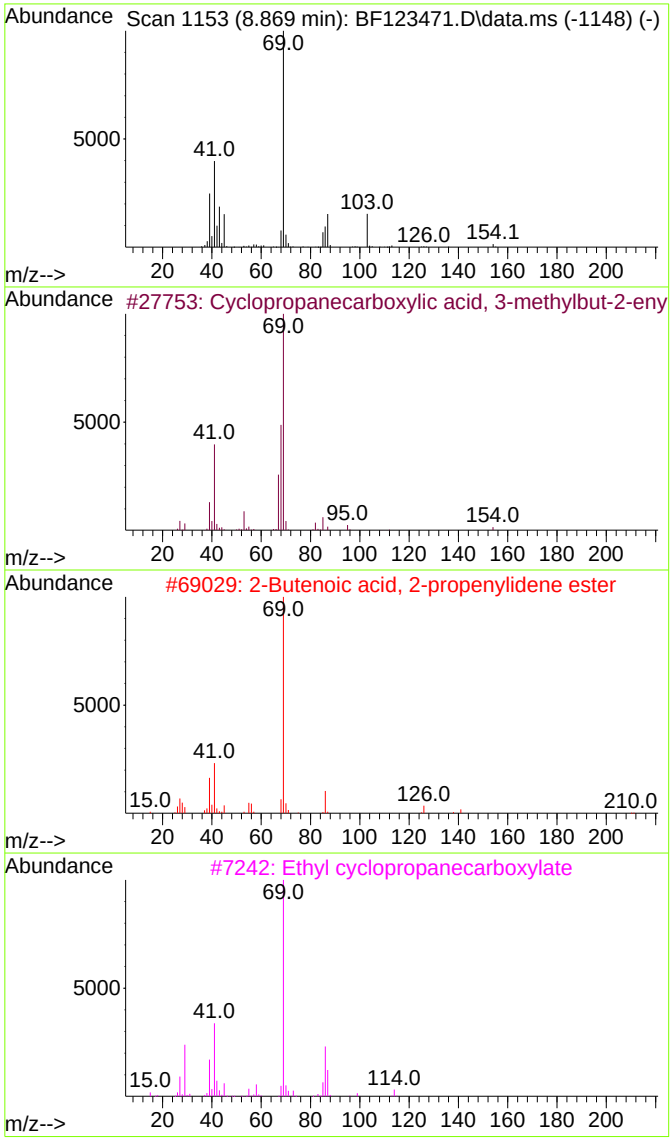
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

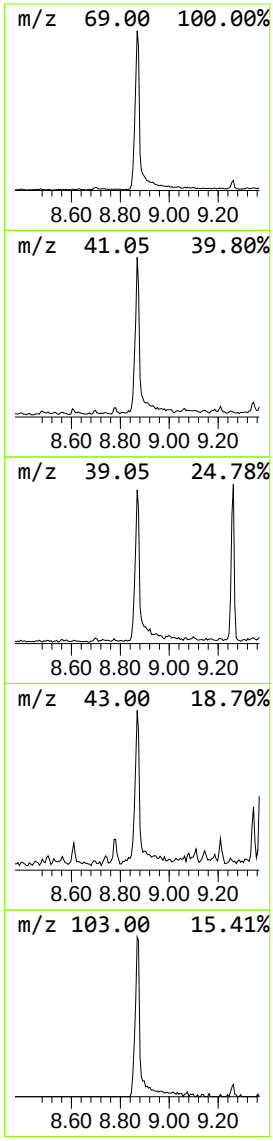
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	7.18 ng	605675	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	50
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
4	Oxazole	69	C3H3NO	000288-42-6	33
5	Isoxazole	69	C3H3NO	000288-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

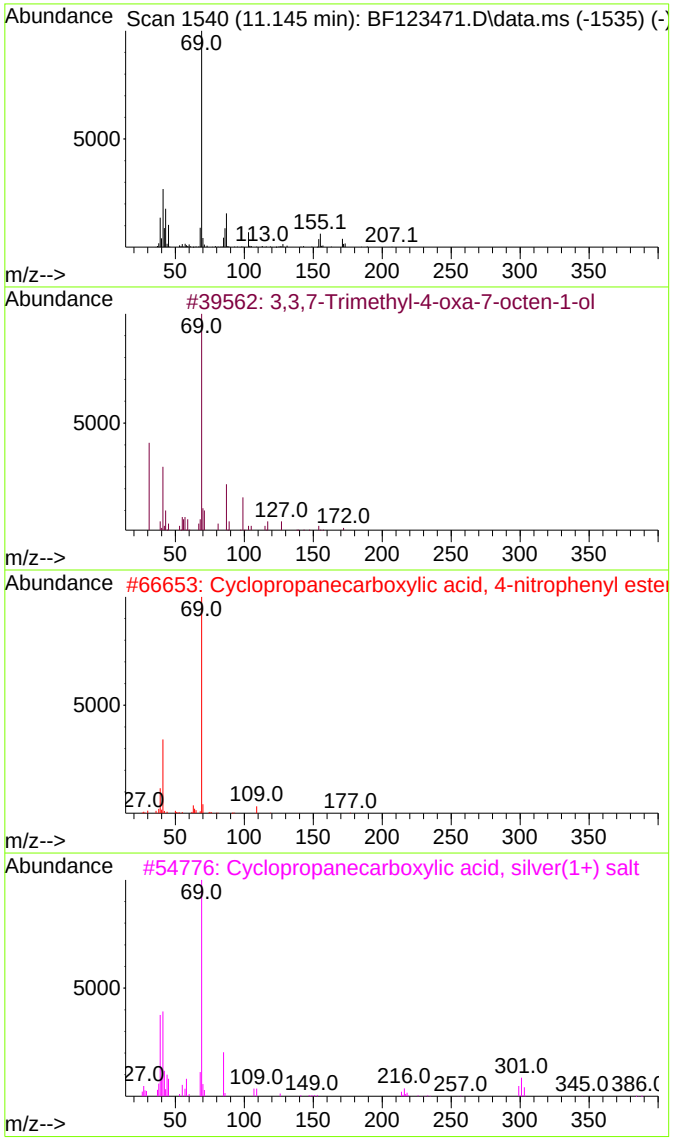
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

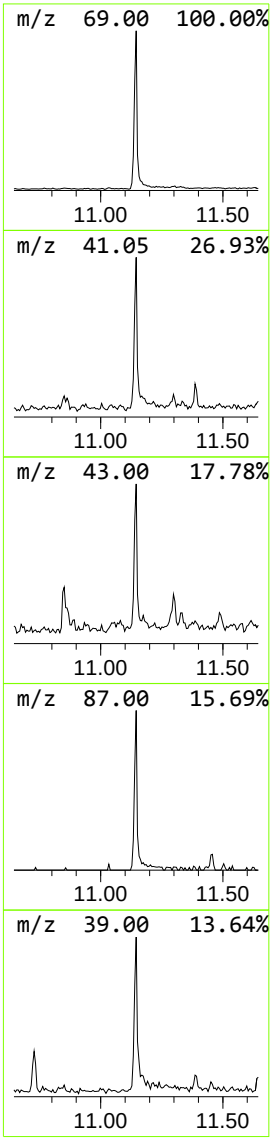
****

Peak Number 3 unknown11.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.145	4.87 ng	340201	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	38
2	Cyclopropanecarboxylic acid, 4-n...	207	C10H9NO4	1000307-52-7	38
3	Cyclopropanecarboxylic acid, sil...	192	C4H5AgO2	075112-77-5	36
4	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
5	Crotonic anhydride	154	C8H10O3	000623-68-7	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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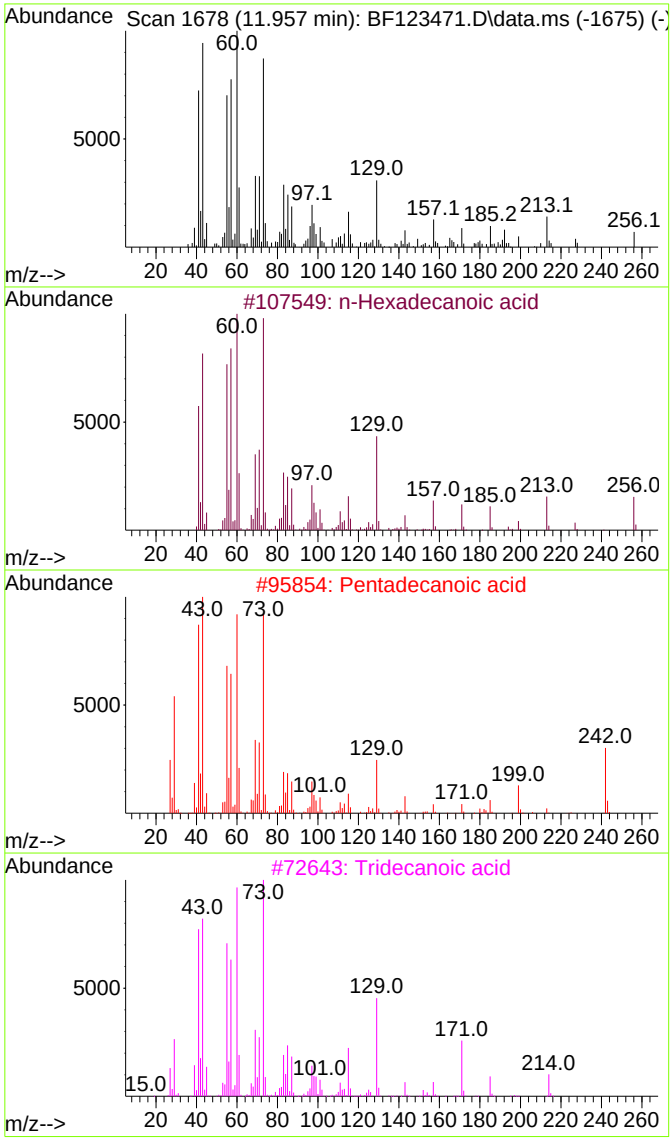
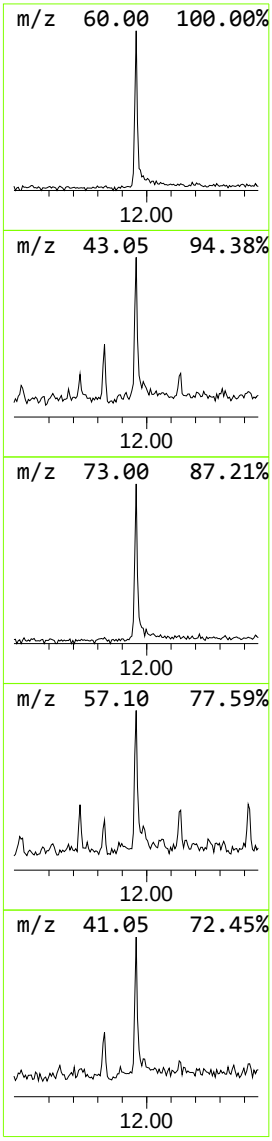
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.80 ng	196080	Phenanthrene-d10	11.433

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	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

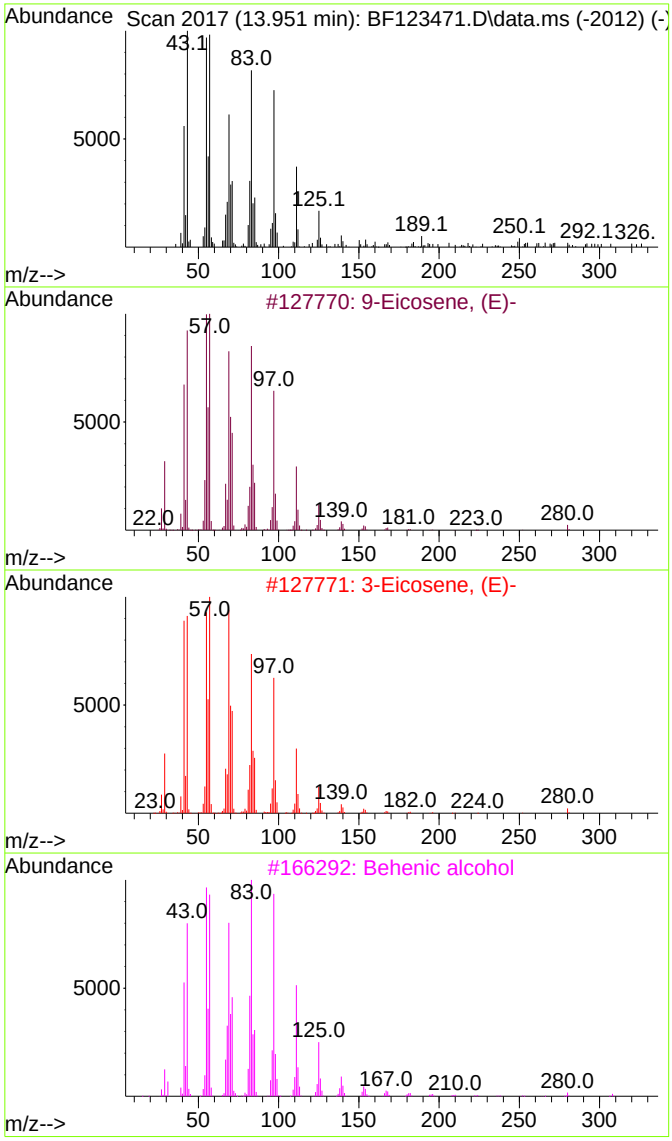
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

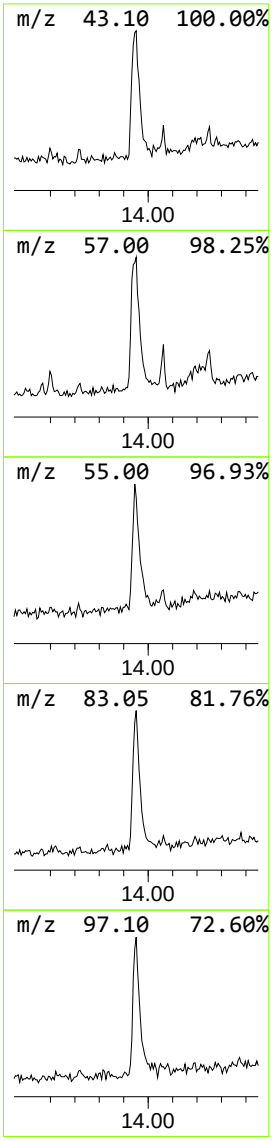
****

Peak Number 5 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	5.48 ng	414087	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

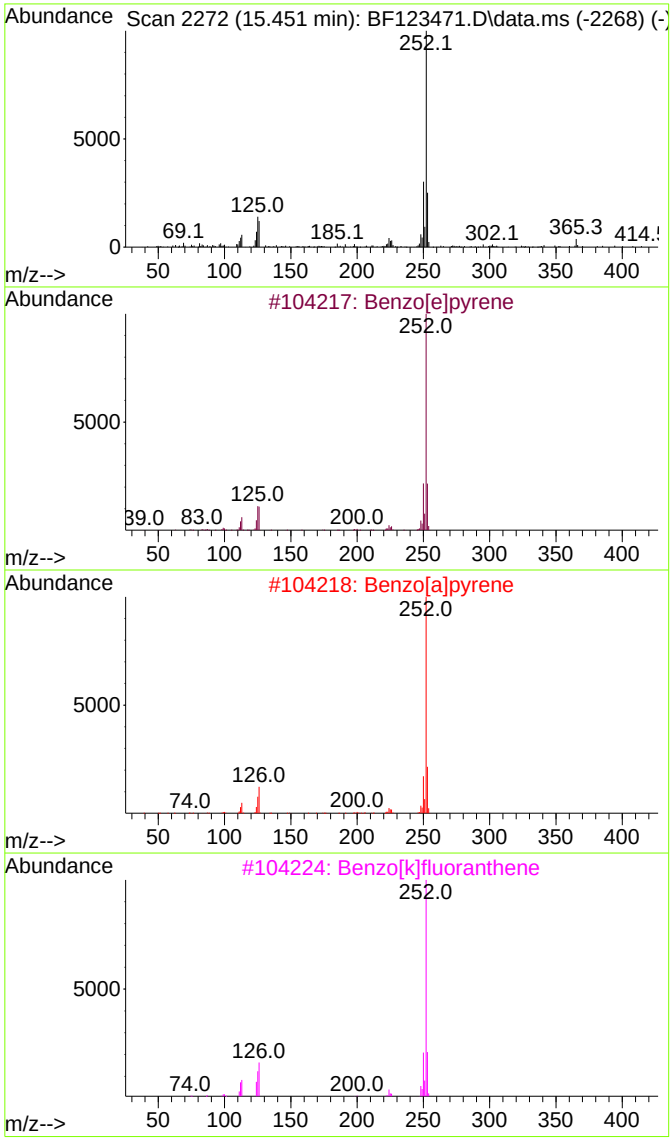
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

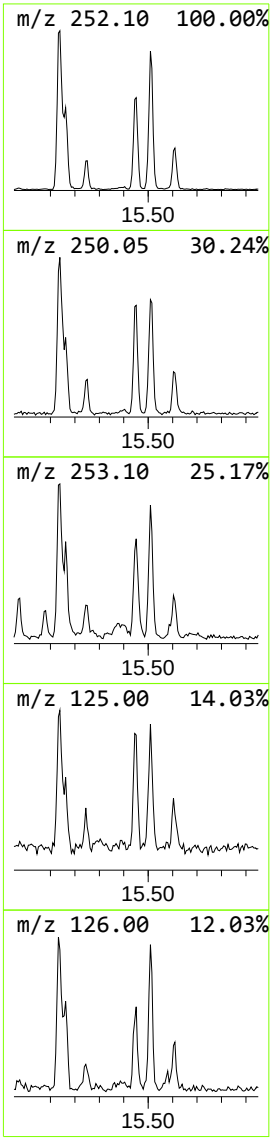
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	5.87 ng	270645	Perylene-d12	15.580

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	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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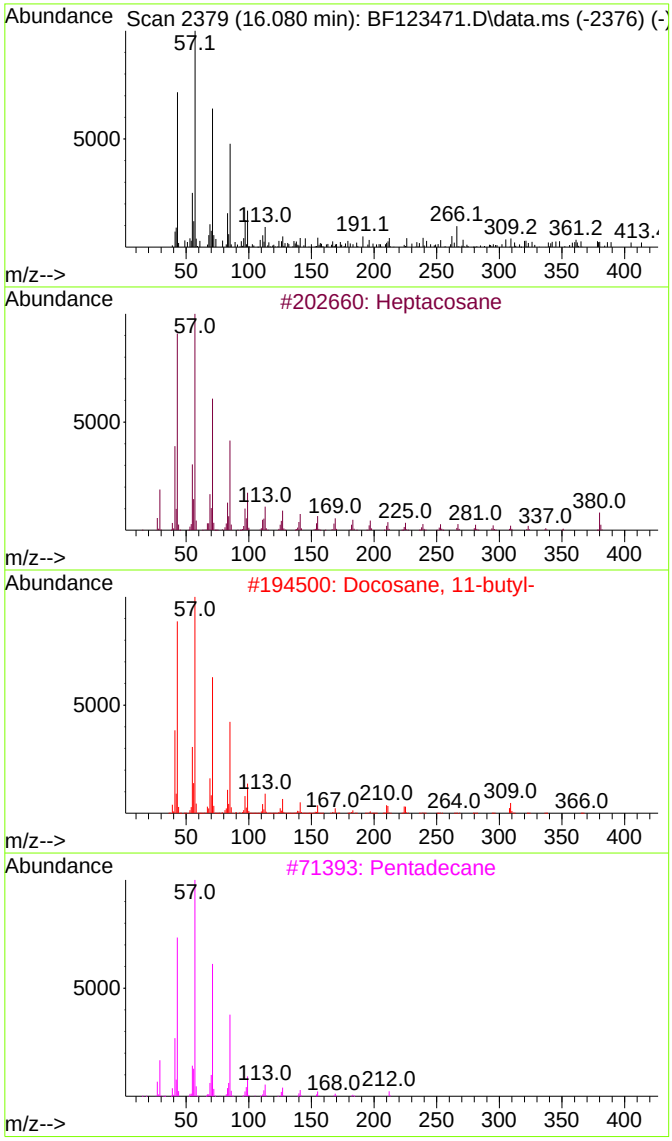
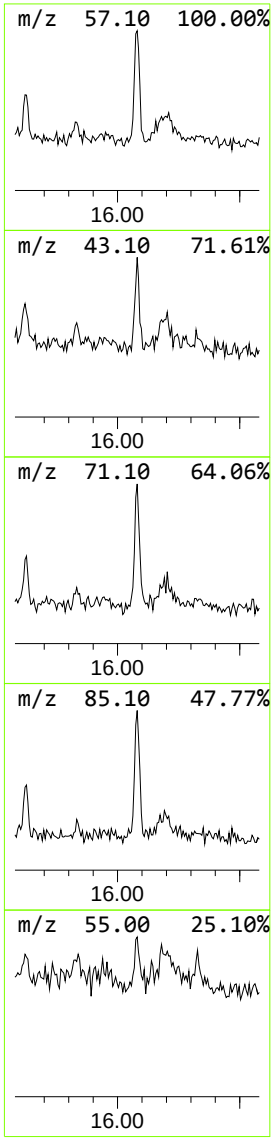
Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	2.38 ng	109801	Perylene-d12	15.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	89
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Hexadecane	226	C16H34	000544-76-3	70
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032521\
Data File : BF123471.D
Acq On : 25 Mar 2021 20:23
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.216	21.2	ng	1400540	1	6.898	1323380	20.0
Cyclopropanecar...	8.869	7.2	ng	605675	2	8.186	1686750	20.0
unknown11.145	11.145	4.9	ng	340201	4	11.433	1398090	20.0
n-Hexadecanoic ...	11.957	2.8	ng	196080	4	11.433	1398090	20.0
9-Eicosene, (E)-	13.951	5.5	ng	414087	5	14.080	1512380	20.0
Benzo[e]pyrene	15.451	5.9	ng	270645	6	15.580	922456	20.0
Heptacosane	16.080	2.4	ng	109801	6	15.580	922456	20.0