LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1-(150.00)

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125187.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	27	rVB	626859	776068	25.50%	2.356%
2	5.134	514	518	526	rVB	79416	93345	3.07%	0.283%
3	5.528	580	585	589	rBV	2911917	2764657	90.83%	8.393%
4	6.534	751	756	759	rBV	2988836	2799004	91.96%	8.498%
5	6.916	817	821	824	rBV	994987	867981	28.52%	2.635%
6	7.475	911	916	919	rBV	2142241	1846951	60.68%	5.607%
7	8.092	1018	1021	1035	rBV	571966	638798	20.99%	1.939%
8	8.198	1035	1039	1041	rVV	1350248	1166002	38.31%	3.540%
9	8.216	1041	1042	1046	rVB	61593	40635	1.34%	0.123%
10	9.269	1217	1221	1224	rBV	3750712	3043709	100.00%	9.241%
11	9.663	1285	1288	1291	rBV	74588	70754	2.32%	0.215%
12	9.810	1307	1313	1318	rBV	46747	41594	1.37%	0.126%
13	9.951	1333	1337	1340	rBV	1630554	1298881	42.67%	3.943%
14	10.151	1366	1371	1375	rBV	42652	43722	1.44%	0.133%
15	10.739	1467	1471	1474	rBV	2452655	2176569	71.51%	6.608%
16	11.239	1553	1556	1560	rBV	43692	38585	1.27%	0.117%
17	11.439	1586	1590	1592	rBV	1567127	1316338	43.25%	3.996%
18	11.457	1592	1593	1597	rVV	170282	133035	4.37%	0.404%
19	11.510	1600	1602	1604	rVV	73524	59071	1.94%	0.179%
20	11.533	1604	1606	1611	rVB3	32811	36412	1.20%	0.111%
21	11.663	1623	1628	1631	rBV2	65960	68683	2.26%	0.209%
22	11.822	1652	1655	1658	rVB	67340	54853	1.80%	0.167%
23	11.880	1661	1665	1670	rBV4	40683	45793	1.50%	0.139%
24	11.957	1671	1678	1683	rBV2	638533	643330	21.14%	1.953%
25	11.998	1683	1685	1690	rVB4	36076	47103	1.55%	0.143%
26	12.051	1690	1694	1696	rBV2	40946	42580	1.40%	0.129%
27	12.139	1702	1709	1711	rBV6	19023	37642	1.24%	0.114%
28	12.257	1726	1729	1732	rVB	60196	53913	1.77%	0.164%
29	12.410	1753	1755	1758	rBV2	52842	40637	1.34%	0.123%
30	12.486	1766	1768	1772	rVB	42619	36117	1.19%	0.110%
31	12.522	1772	1774	1780	rBV5	23297	36659	1.20%	0.111%
32	12.574	1780	1783	1788	rVB	51945	53178	1.75%	0.161%
33	12.651	1792	1796	1802	rBV	674481	624693	20.52%	1.897%
34	12.739	1808	1811	1815	rBV2	141898	133128	4.37%	0.404%
35	12.880	1832	1835	1840	rVB	657571	563037	18.50%	1.709%
36	12.927	1840	1843	1849	rVB3	39574	52200	1.72%	0.158%

LSC Area Percent Report

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Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1-(150.00)

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.021	1855	1859	1866	rVB	3044752	2834947	93.14%	8.607%
38	13.098	1867	1872	1875	rBV3	60123	91934	3.02%	0.279%
39	13.186	1880	1887	1888	rBV4	59378	91403	3.00%	0.277%
40	13.204	1888	1890	1894	rVB	73074	71765	2.36%	0.218%
41	13.239	1894	1896	1899	rBV2	29506	36553	1.20%	0.111%
42	13.310	1904	1908	1911	rVB2	94691	95337	3.13%	0.289%
43	13.404	1921	1924	1927	rBV	52219	49939	1.64%	0.152%
44	13.433	1927	1929	1933	rBV2	45416	50183	1.65%	0.152%
45	13.592	1952	1956	1957	rBV4	36089	45012	1.48%	0.137%
46	13.633	1961	1963	1966	rVV	87602	66857	2.20%	0.203%
47	13.710	1973	1976	1982	rVB	141899	144121	4.74%	0.438%
48	13.827	1992	1996	1999	rBV2	91980	116408	3.82%	0.353%
49	13.857	1999	2001	2003	rBV	86611	81240	2.67%	0.247%
50	13.880	2003	2005	2008	rVB2	96589	86958	2.86%	0.264%
51	13.921	2008	2012	2014	rBV2	113392	104236	3.42%	0.316%
52	13.945	2014	2016	2017	rBV	65000	52905	1.74%	0.161%
53	13.968	2018	2020	2024	rBV3	47359	65862	2.16%	0.200%
54	14.080	2030	2039	2041	rBV2	1126041	1448656	47.60%	4.398%
55	14.104	2041	2043	2049	rVB	489528	428426	14.08%	1.301%
56	14.292	2072	2075	2080	rBV4	42724	65079	2.14%	0.198%
57	14.463	2100	2104	2107	rVB	89486	106937	3.51%	0.325%
58	14.498	2107	2110	2114	rBV2	107350	113416	3.73%	0.344%
59	14.545	2114	2118	2123	rBV6	57780	95343	3.13%	0.289%
60	14.592	2123	2126	2128	rBV	57719	68303	2.24%	0.207%
61	14.663	2136	2138	2143	rVB2	52566	57983	1.91%	0.176%
62	14.774	2154	2157	2160	rBV	48791	64045	2.10%	0.194%
63	14.939	2181	2185	2189	rBV2	165793	206462	6.78%	0.627%
64	15.039	2199	2202	2204	rVB2	42429	40668	1.34%	0.123%
65	15.133	2213	2218	2221	rBV	588846	855032	28.09%	2.596%
66	15.210	2228	2231	2234	rVV2	54000	60892	2.00%	0.185%
67	15.245	2234	2237	2241	rVB	69982	70482	2.32%	0.214%
68	15.339	2250	2253	2256	rBV4	32781	41773	1.37%	0.127%
69	15.445	2267	2271	2278	rVB	321416	412389	13.55%	1.252%
70	15.510	2278	2282	2288	rBV	212308	254636	8.37%	0.773%
71	15.574	2288	2293	2297	rBV	768638	1002739	32.94%	3.044%
72	16.057	2372	2375	2380	rVB4	36766	49816	1.64%	0.151%
73	17.080	2543	2549	2555	rVB2	141336	266773	8.76%	0.810%
74	17.145	2555	2560	2566	rBV2	111229	194673	6.40%	0.591%
75	17.333	2587	2592	2595	rBV4	22216	40775	1.34%	0.124%
76	17.533	2621	2626	2632	rVB	113578	209376	6.88%	0.636%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
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Acq On : 24 Aug 2021 16:11
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Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	18.286	2747	2754	2764	rVB7	135385	329889	10.84%	1.002%
78	18.603	2797	2808	2814	rBV7	134239	582542	19.14%	1.769%

Sum of corrected areas: 32938422

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
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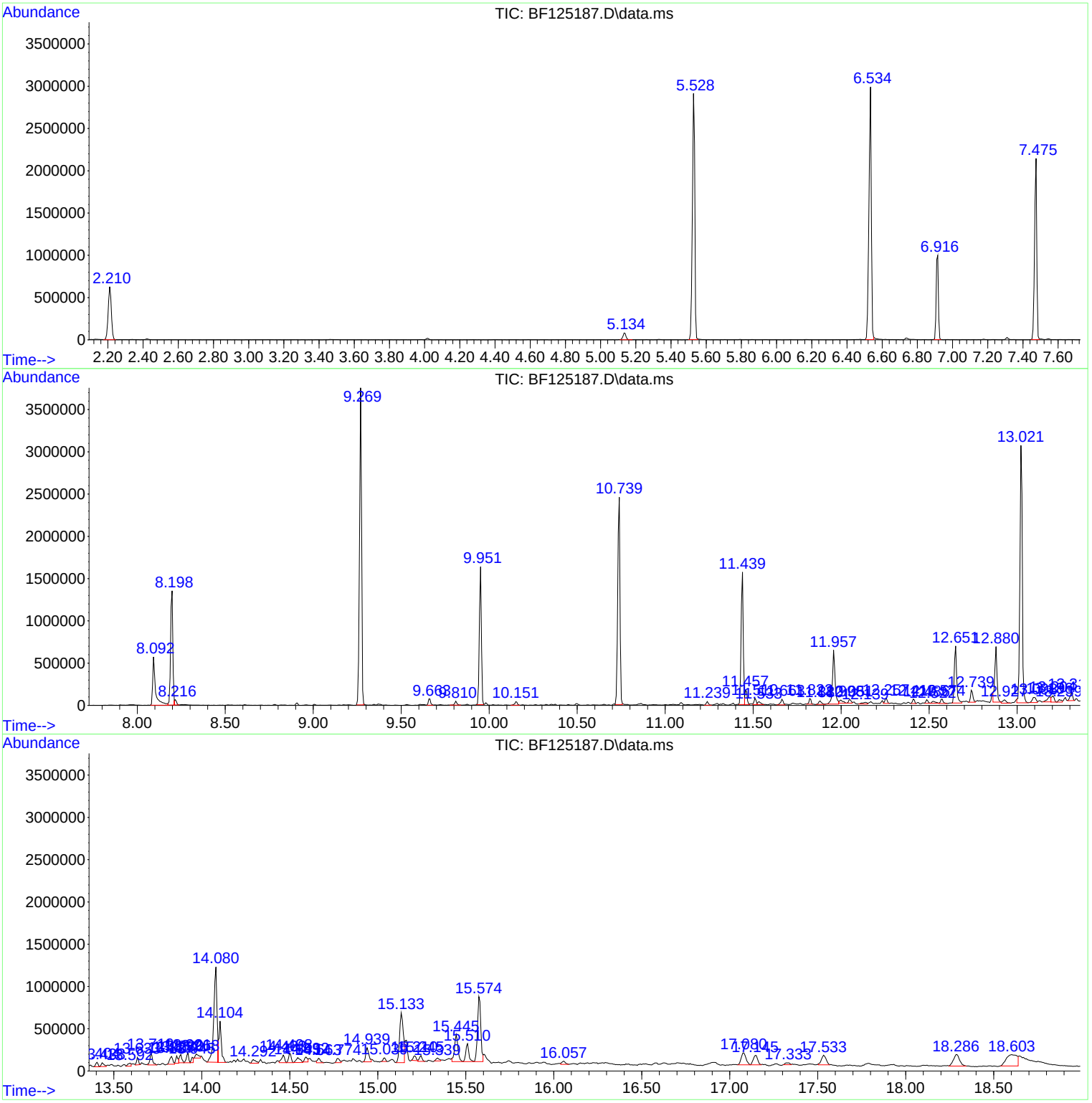
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

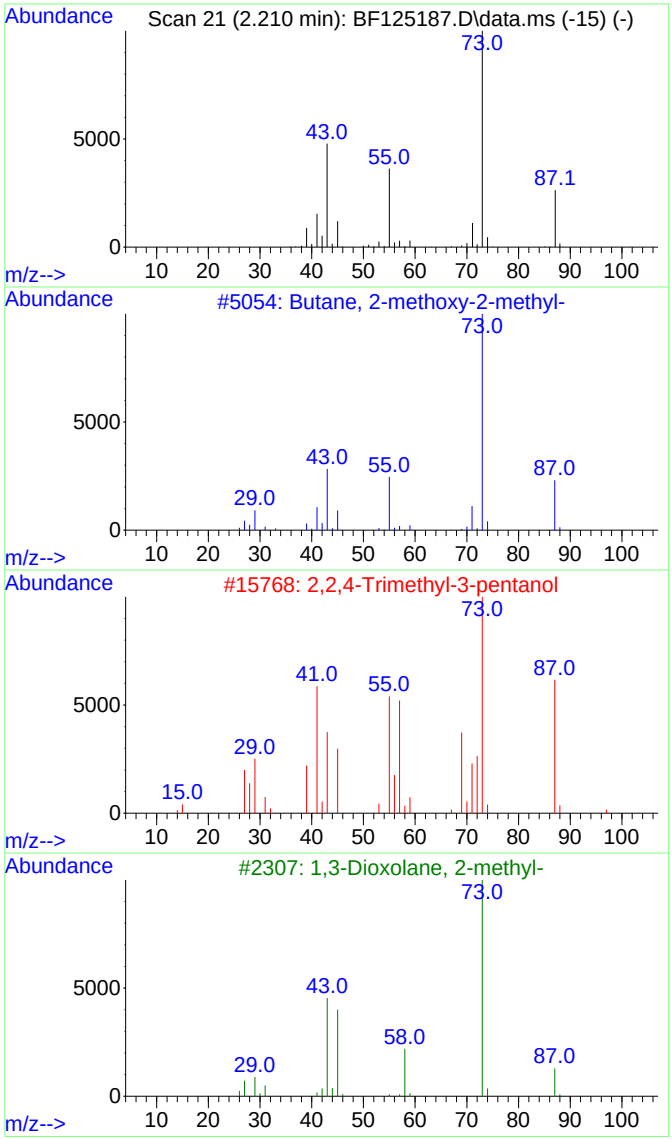
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

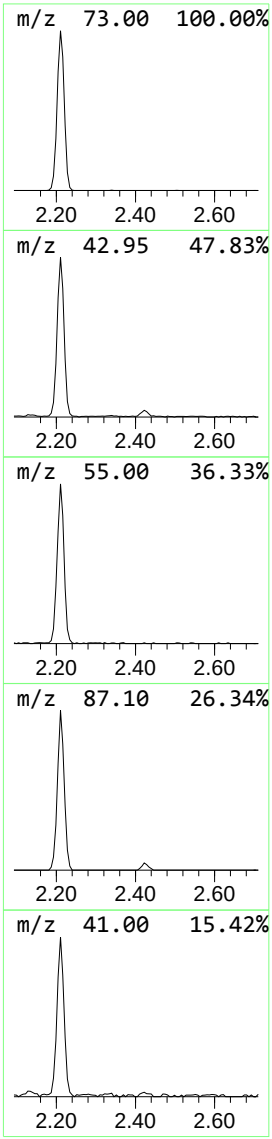
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	17.88 ng	776068	1,4-Dichlorobenzene-d4	6.916

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
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Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

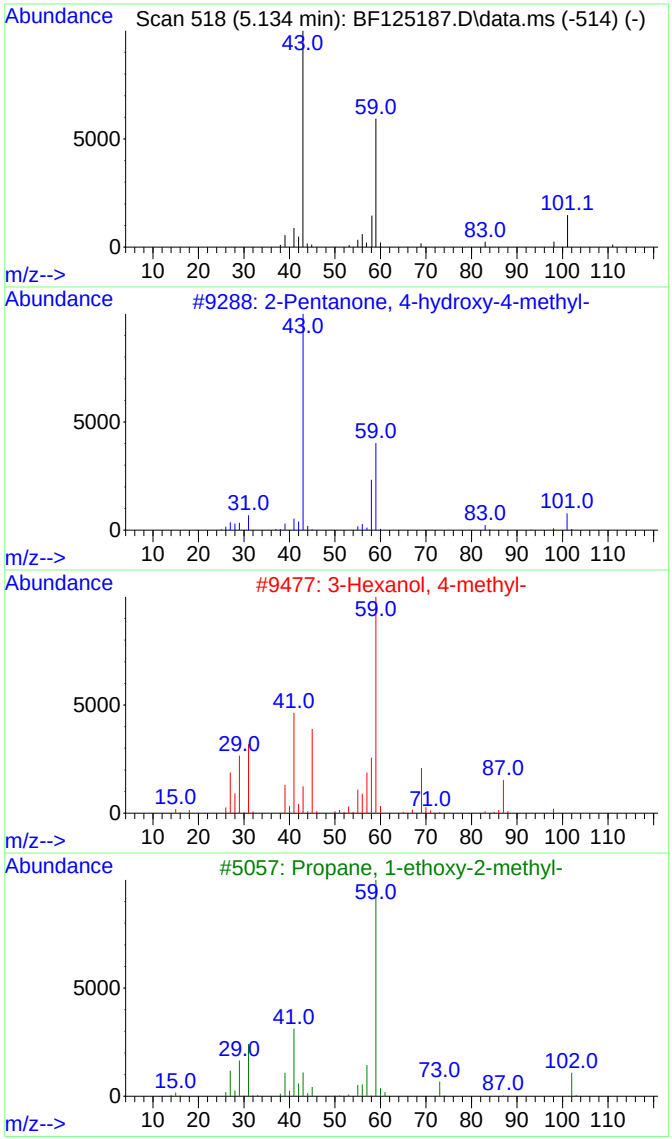
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

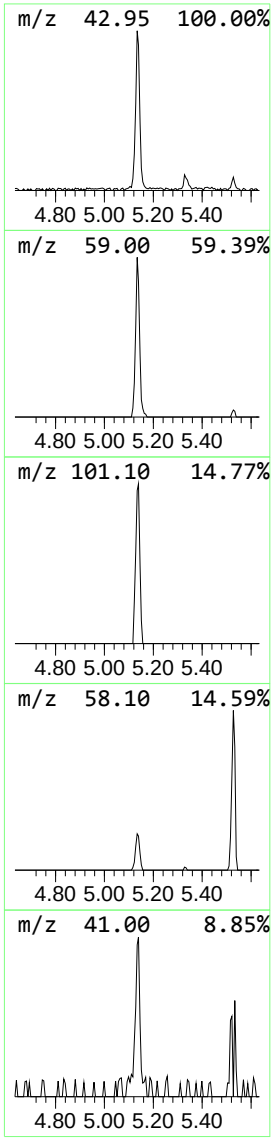
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	2.15 ng	93345	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
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Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1-(150.00)

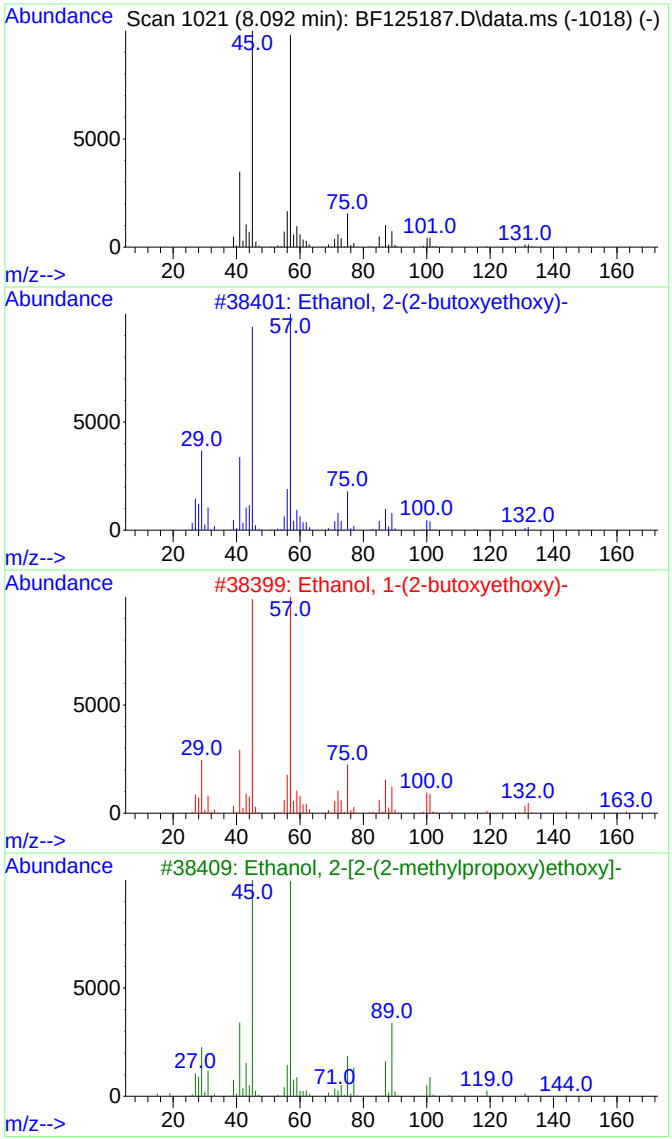
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

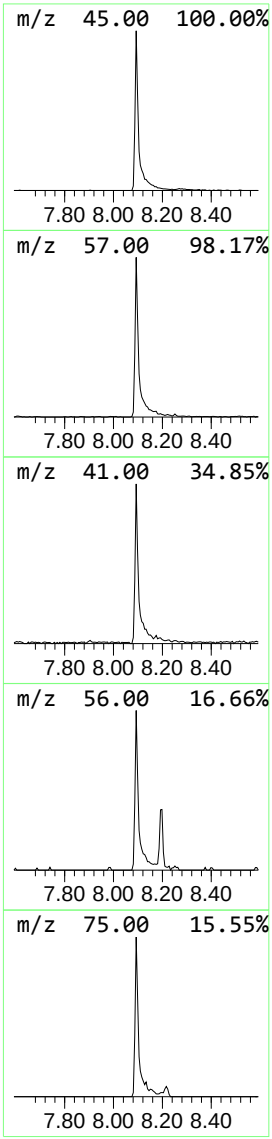
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	10.96 ng	638798	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	(S)-Methyl 2,3-dihydroxypropanoa...	134	C5H10O4	354578-58-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
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SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

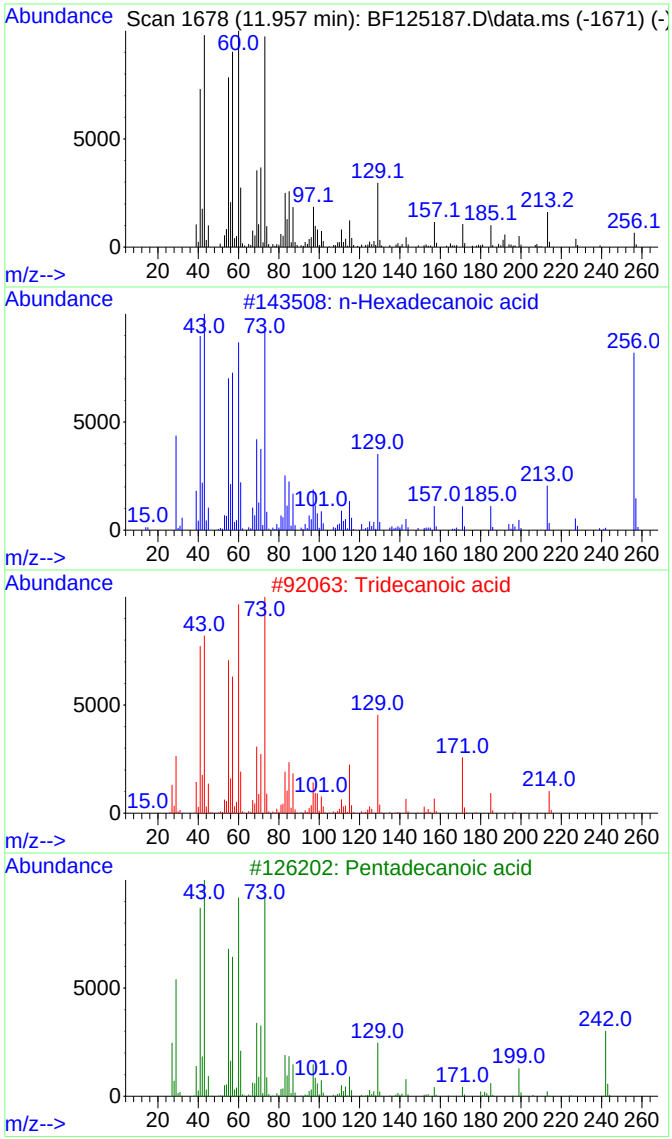
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

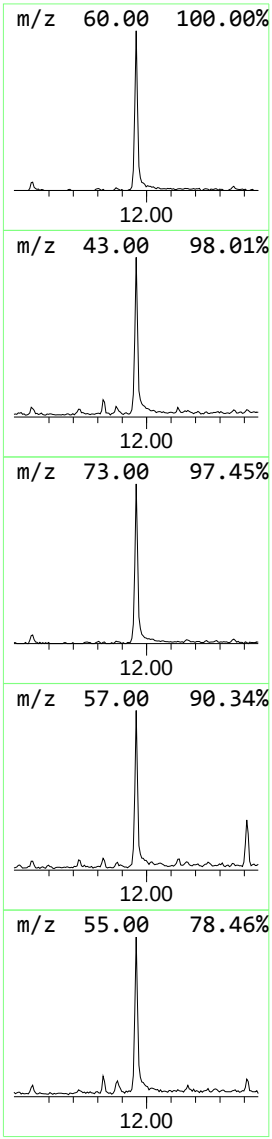
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	9.77 ng	643330	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Acq On : 24 Aug 2021 16:11
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Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

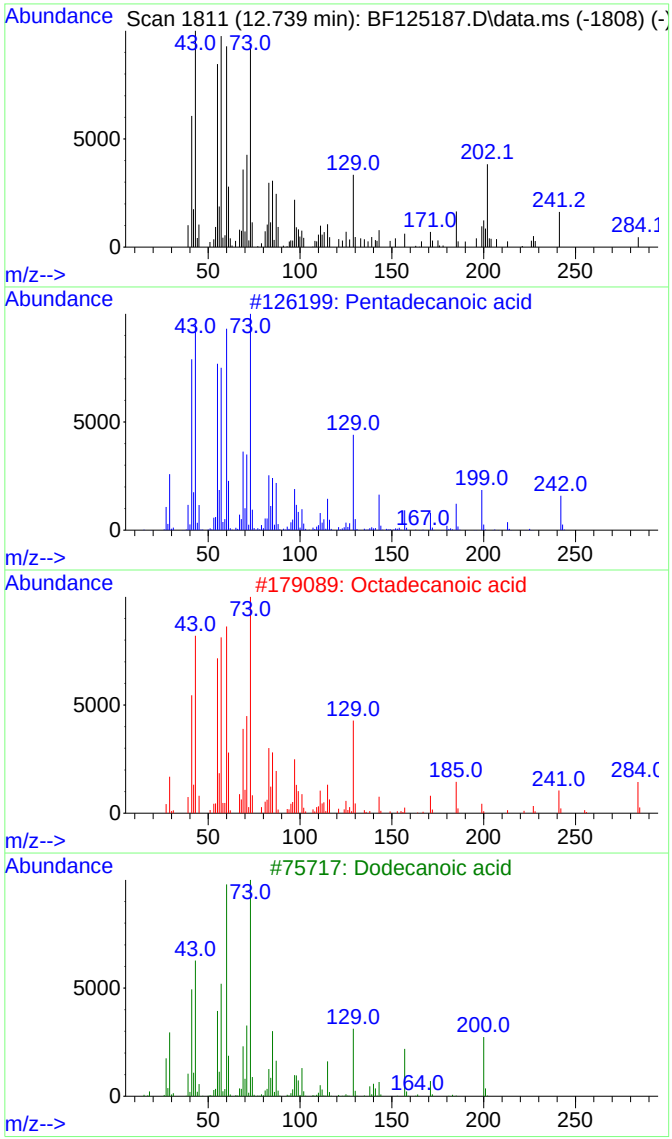
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

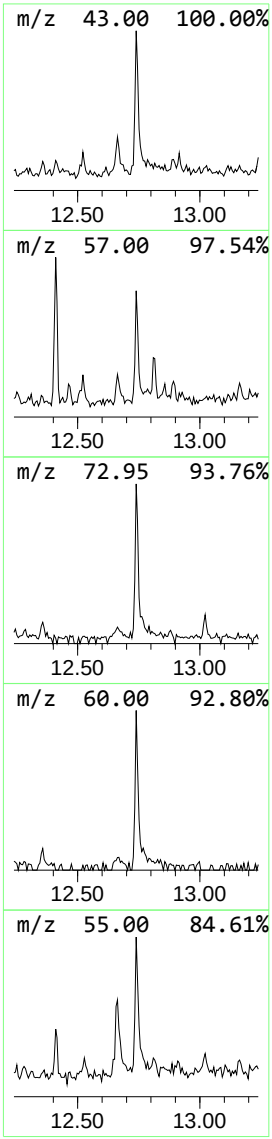
****

Peak Number 5 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.02 ng	133128	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	Octadecanoic acid	284	C18H36O2	000057-11-4	72
3	Dodecanoic acid	200	C12H24O2	000143-07-7	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

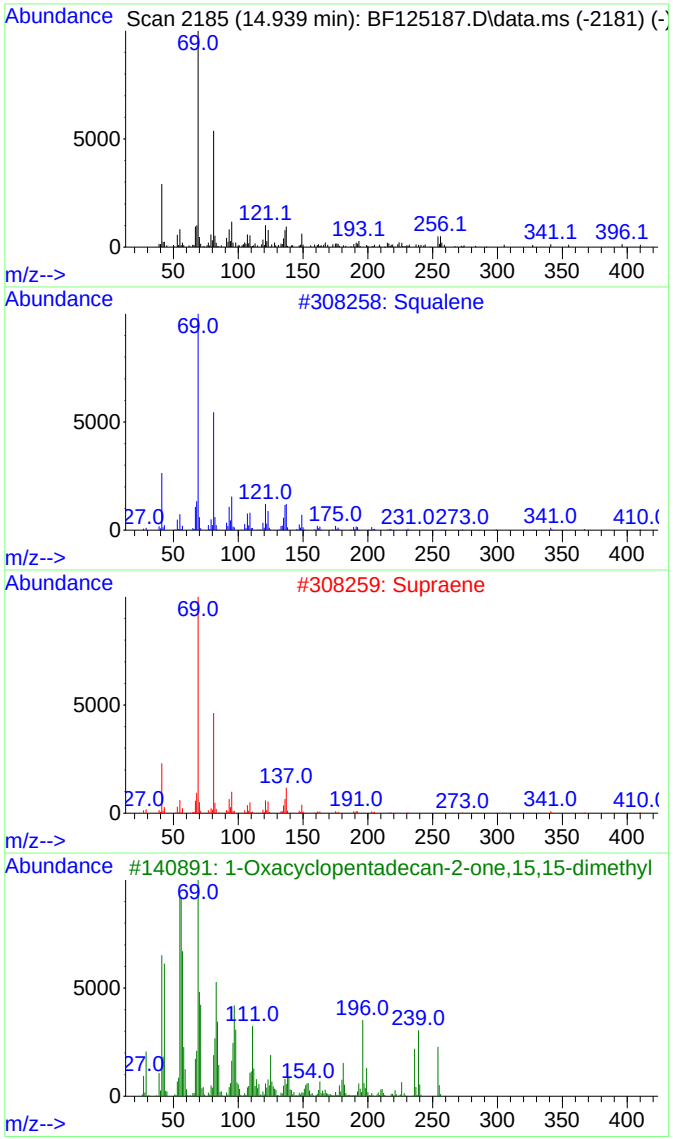
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

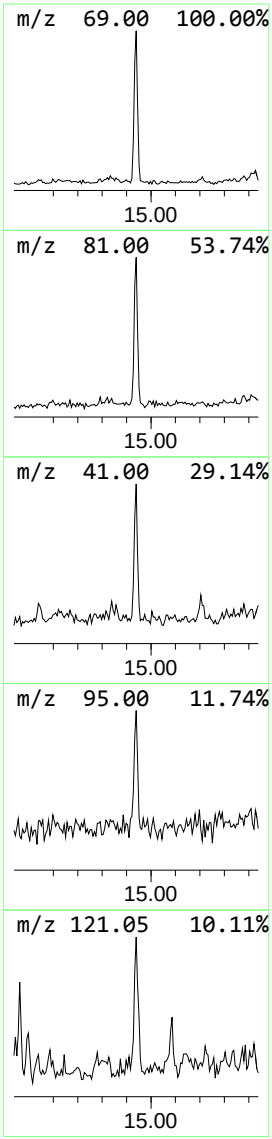
****

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	4.12 ng	206462	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	96
2	Supraene	410	C30H50	007683-64-9	68
3	1-Oxacyclopentadecan-2-one,15,15...	254	C16H30O2	1000196-63-1	64
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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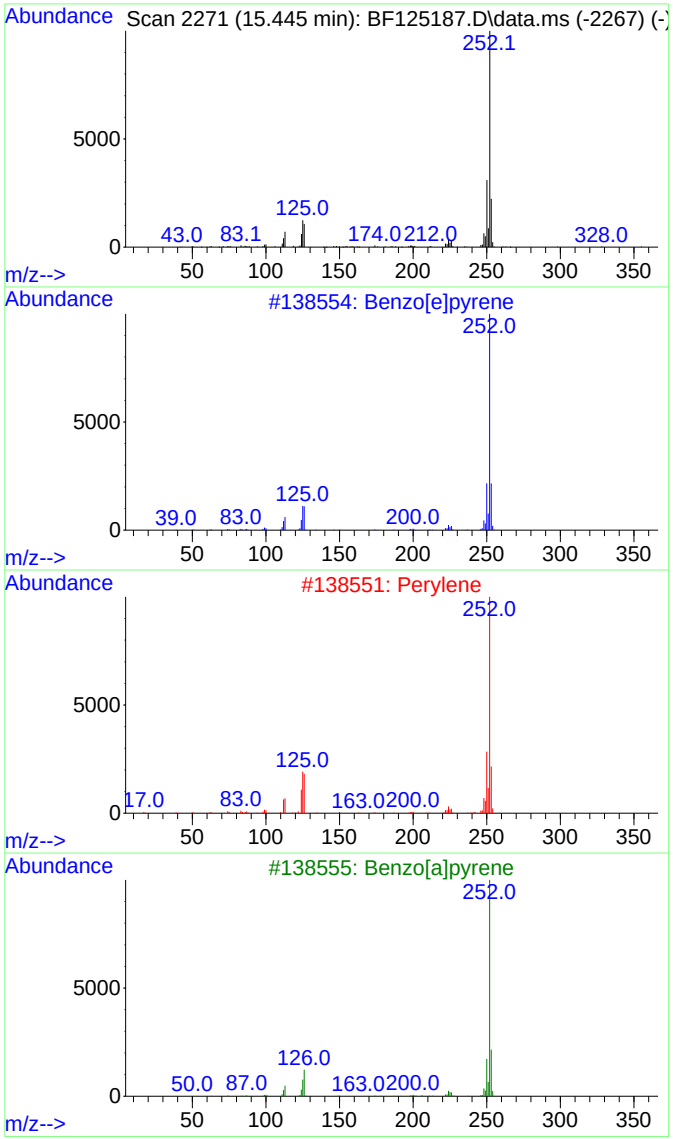
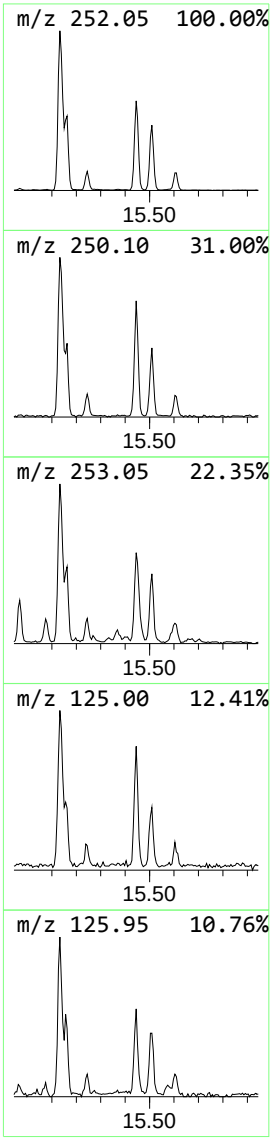
Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	8.23 ng	412389	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





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Data File : BF125187.D
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Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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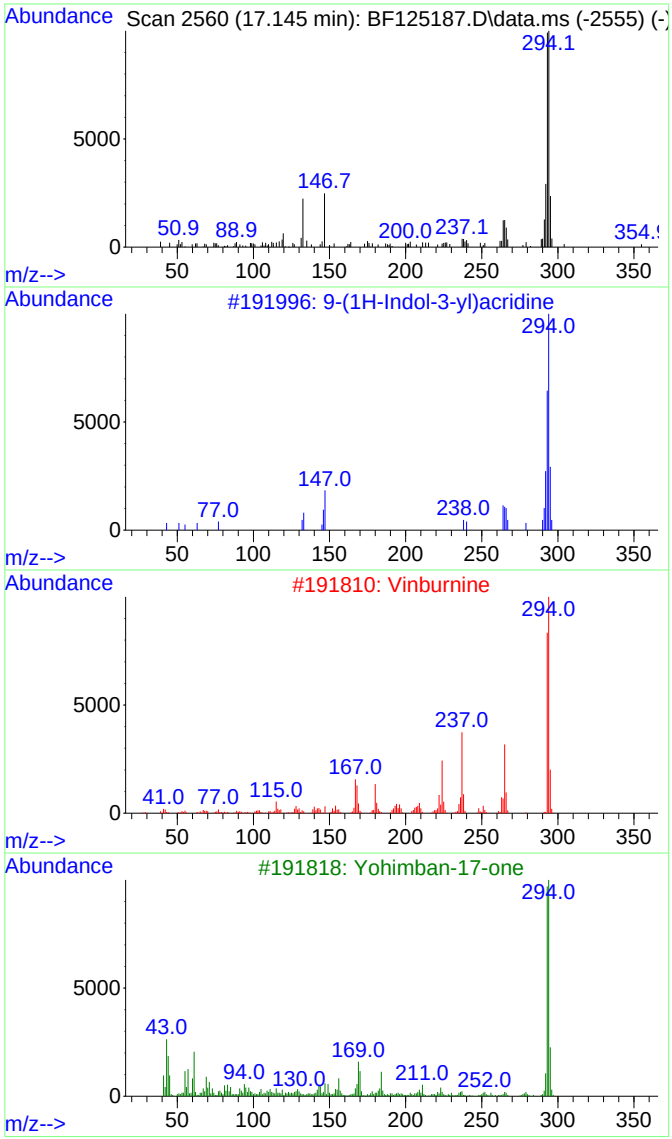
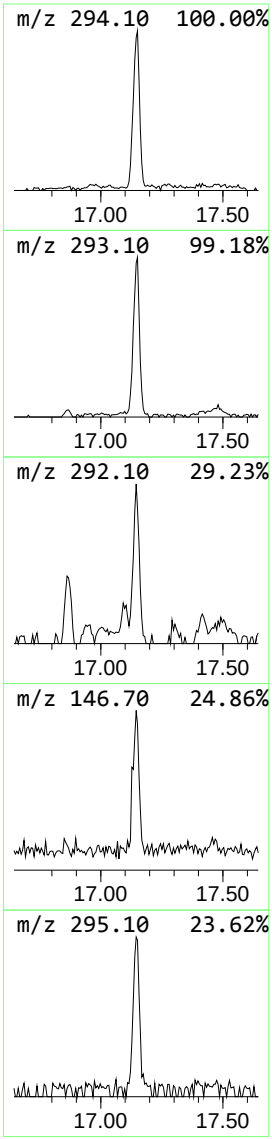
Peak Number 8 9-(1H-Indol-3-yl)acridine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	3.88 ng	194673	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-(1H-Indol-3-yl)acridine	294	C21H14N2	1010326-84-0	91
2	Vinburnine	294	C19H22N2O	004880-88-0	62
3	Yohimban-17-one	294	C19H22N2O	000523-14-8	58
4	Eburnamenin-14(15H)-one, (.+/-.)-	294	C19H22N2O	002580-88-3	53
5	11-Methyldibenzo(a,c)phenazine	294	C21H14N2	004559-60-8	43





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Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

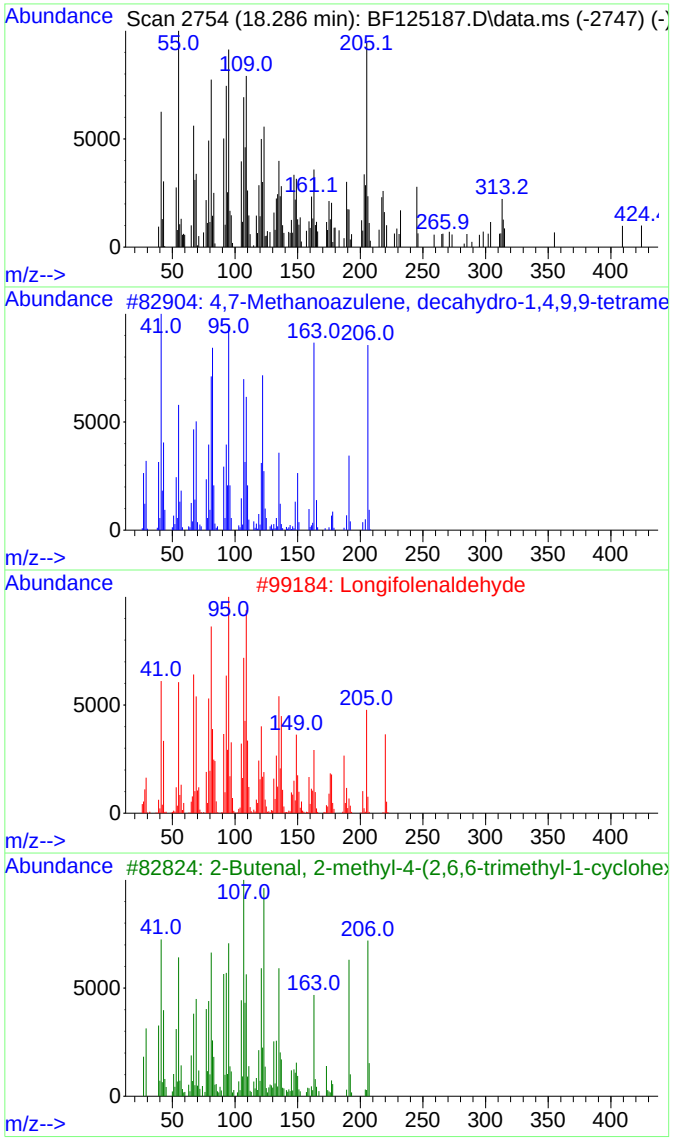
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

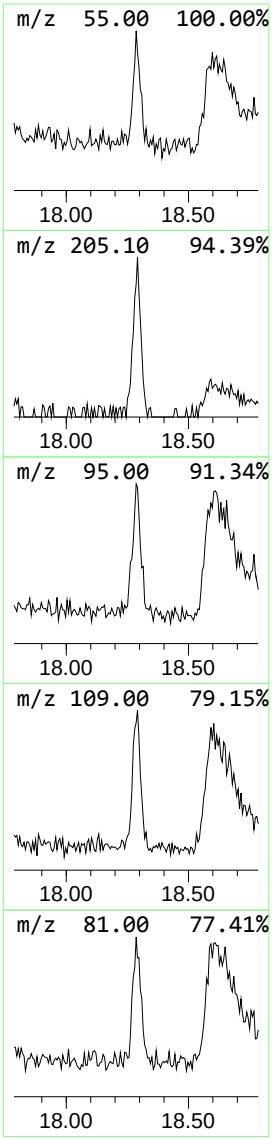
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4,7-Methanoazulene, decahyd... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	6.58 ng	329889	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	53
2	Longifolenaldehyde	220	C15H24O	019890-84-7	49
3	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	41
4	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	40
5	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1-(150.00)

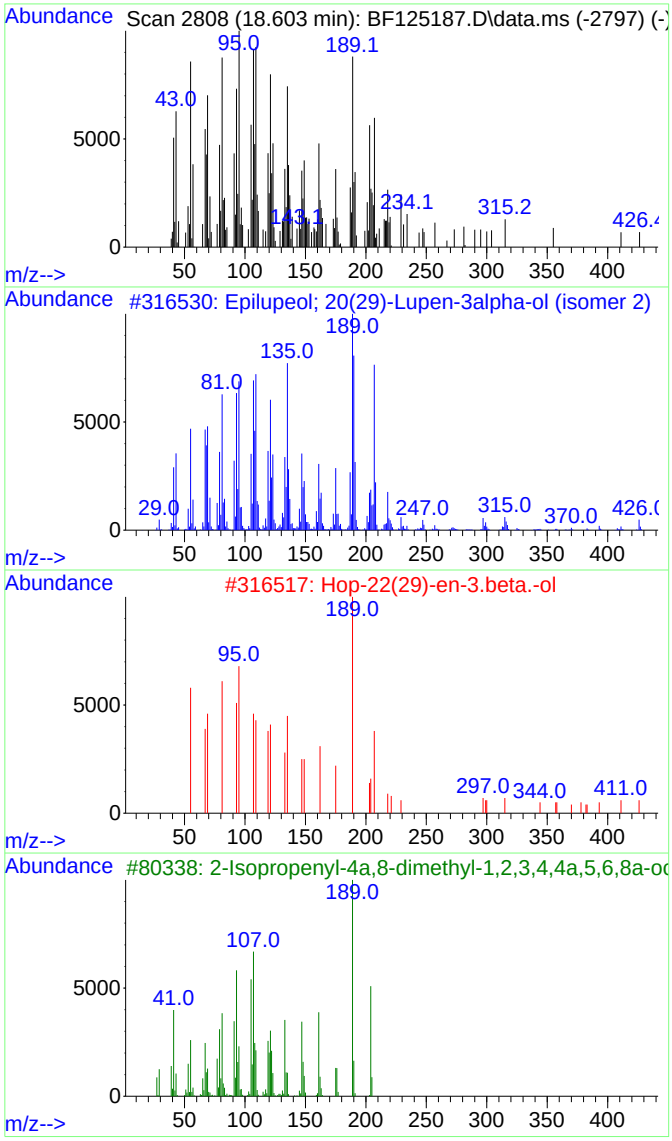
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

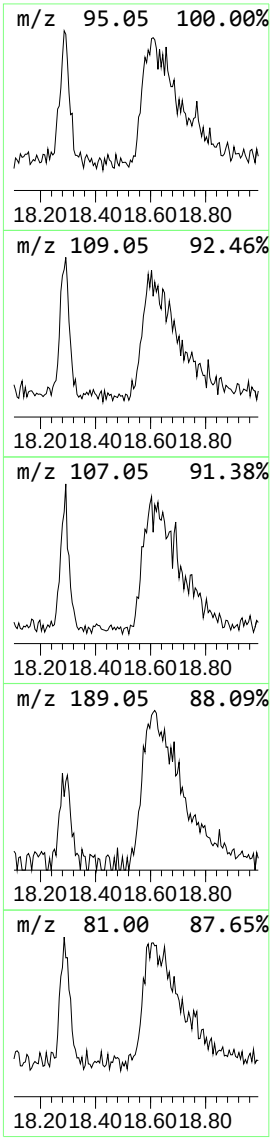
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Epilupeol; 20(29)-Lupen-3al... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.604	11.62 ng	582542	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	94
2	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	84
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	72
4	Squamulosone	218	C15H22O	034413-94-0	62
5	1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125187.D
Acq On : 24 Aug 2021 16:11
Operator : JU/CG
Sample : M3467-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1-(150.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.210	17.9	ng	776068	1	6.916	867981	20.0
2-Pentanone, 4-...	5.134	2.1	ng	93345	1	6.916	867981	20.0
Ethanol, 2-(2-b...	8.092	11.0	ng	638798	2	8.198	1166000	20.0
n-Hexadecanoic ...	11.957	9.8	ng	643330	4	11.439	1316340	20.0
Pentadecanoic acid	12.739	2.0	ng	133128	4	11.439	1316340	20.0
Squalene	14.939	4.1	ng	206462	6	15.574	1002740	20.0
Benzo[e]pyrene	15.445	8.2	ng	412389	6	15.574	1002740	20.0
9-(1H-Indol-3-y...	17.145	3.9	ng	194673	6	15.574	1002740	20.0
4,7-Methanoazul...	18.286	6.6	ng	329889	6	15.574	1002740	20.0
Epilupeol; 20(2...	18.604	11.6	ng	582542	6	15.574	1002740	20.0