LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121522\
Data File : BF131652.D
Acq On : 15 Dec 2022 16:47
Operator : CG\JU
Sample : N6038-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-35-(2.5-4.5)

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	17	rVB	417104	516600	23.95%	3.425%
2	5.093	506	511	519	rVB	208334	257800	11.95%	1.709%
3	5.498	575	580	583	rBV	1985778	1852221	85.87%	12.280%
4	6.510	747	752	755	rBV	1816745	1902301	88.19%	12.612%
5	6.881	811	815	818	rBV	461216	376597	17.46%	2.497%
6	7.445	906	911	914	rBV	1220604	1215652	56.36%	8.060%
7	8.169	1030	1034	1037	rBV	569375	482986	22.39%	3.202%
8	9.251	1212	1218	1221	rBV	2373823	2156996	100.00%	14.301%
9	9.934	1329	1334	1337	rBV	685893	575054	26.66%	3.813%
10	10.651	1452	1456	1459	rBV	286700	222035	10.29%	1.472%
11	10.728	1464	1469	1472	rBV	1775908	1501510	69.61%	9.955%
12	11.428	1584	1588	1590	rBV	756473	623369	28.90%	4.133%
13	11.451	1590	1592	1595	rVB	30289	24129	1.12%	0.160%
14	11.957	1675	1678	1686	rBV2	72057	74399	3.45%	0.493%
15	12.198	1716	1719	1722	rBV	56032	47506	2.20%	0.315%
16	12.645	1791	1795	1798	rBV	50133	46765	2.17%	0.310%
17	12.874	1829	1834	1838	rBV	44236	44656	2.07%	0.296%
18	13.022	1854	1859	1862	rBV	2469881	2133069	98.89%	14.142%
19	13.945	2008	2016	2028	rBV7	37495	173310	8.03%	1.149%
20	14.074	2034	2038	2042	rBV	420440	402345	18.65%	2.668%
21	14.174	2051	2055	2059	rVB	33530	36234	1.68%	0.240%
22	14.939	2180	2185	2189	rBV	36230	39566	1.83%	0.262%
23	15.133	2213	2218	2221	rBV2	16404	26321	1.22%	0.175%
24	15.580	2289	2294	2302	rBV	295663	351676	16.30%	2.332%

Sum of corrected areas: 15083097

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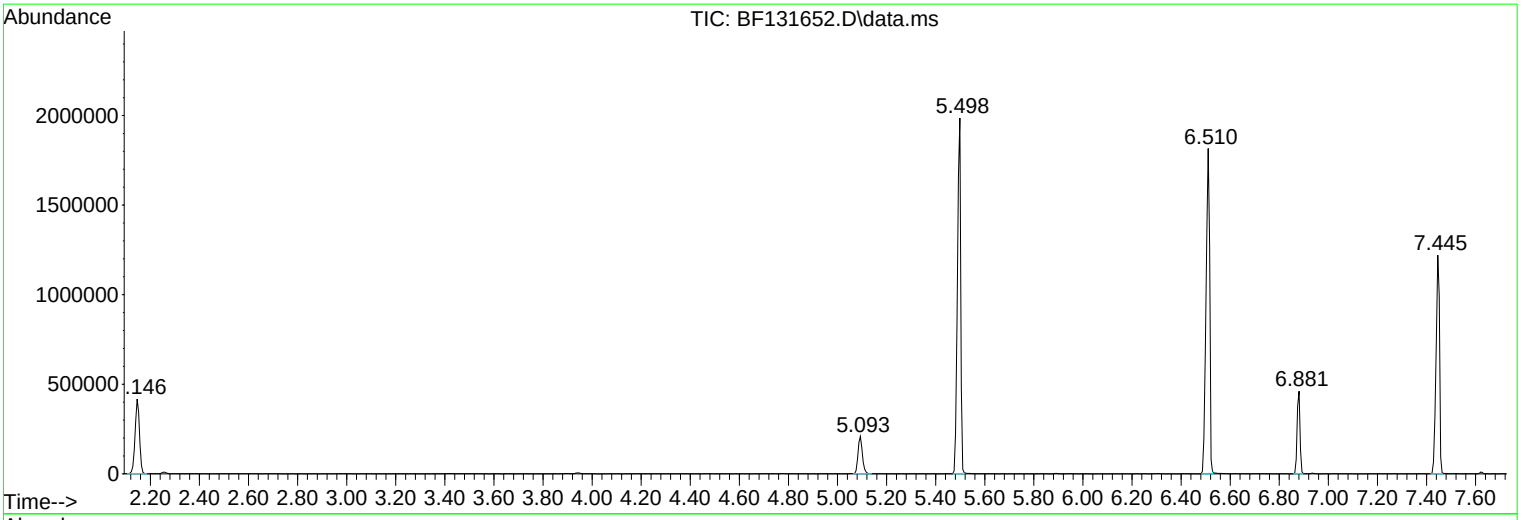
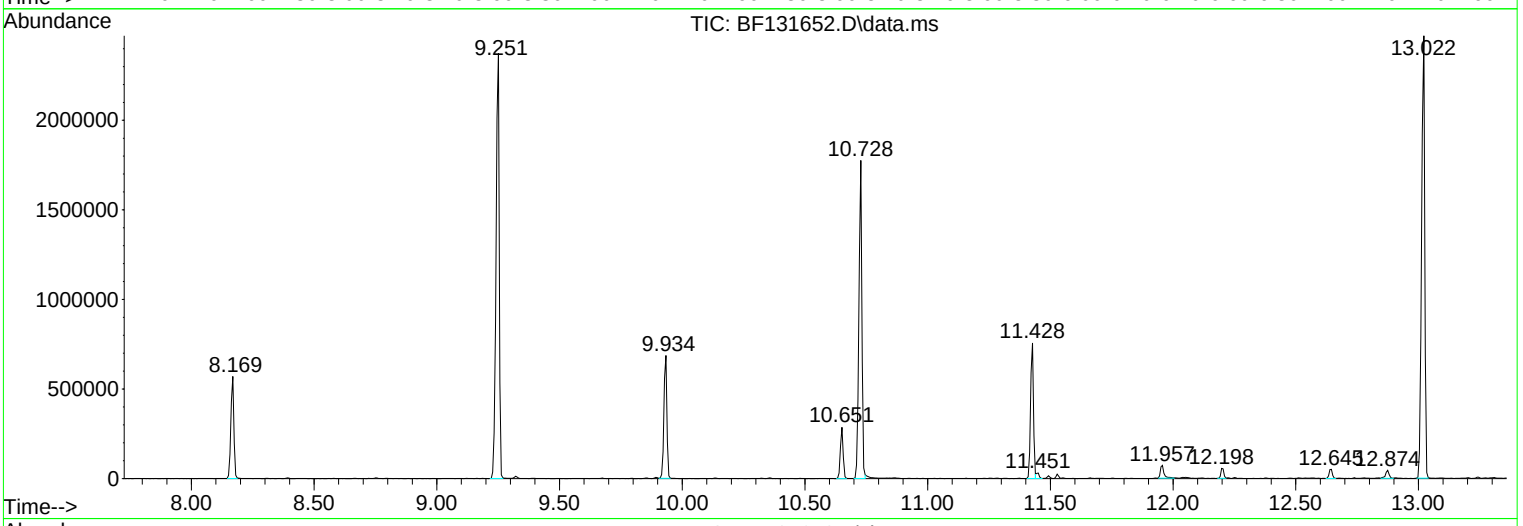
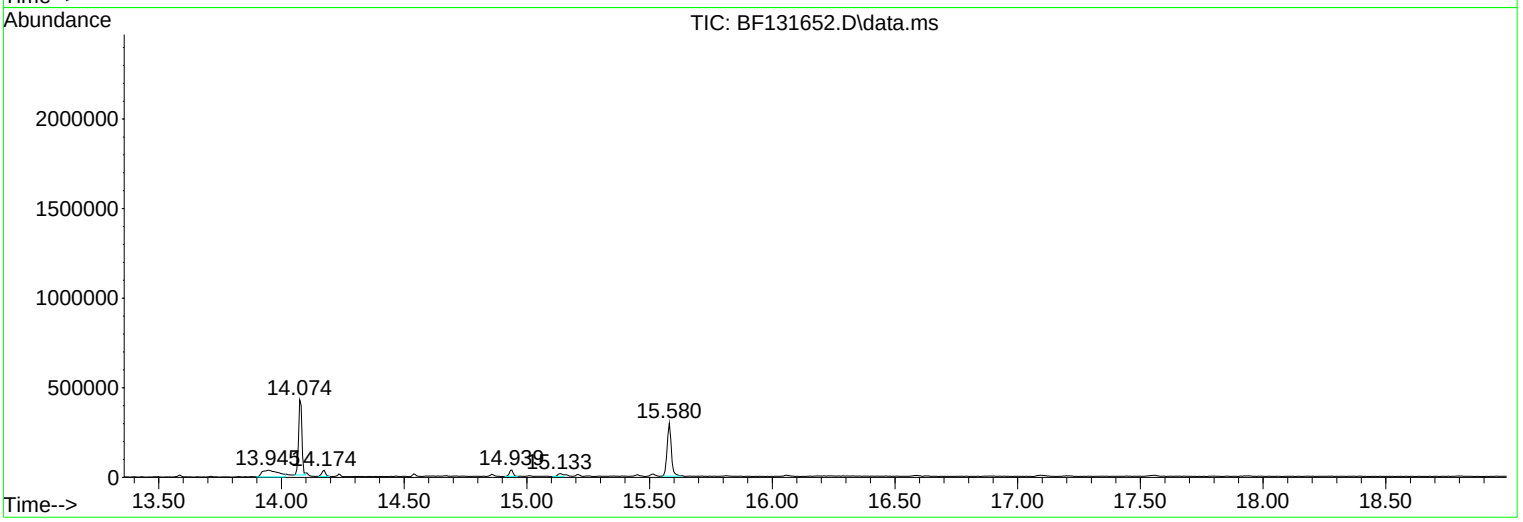
RB-35-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

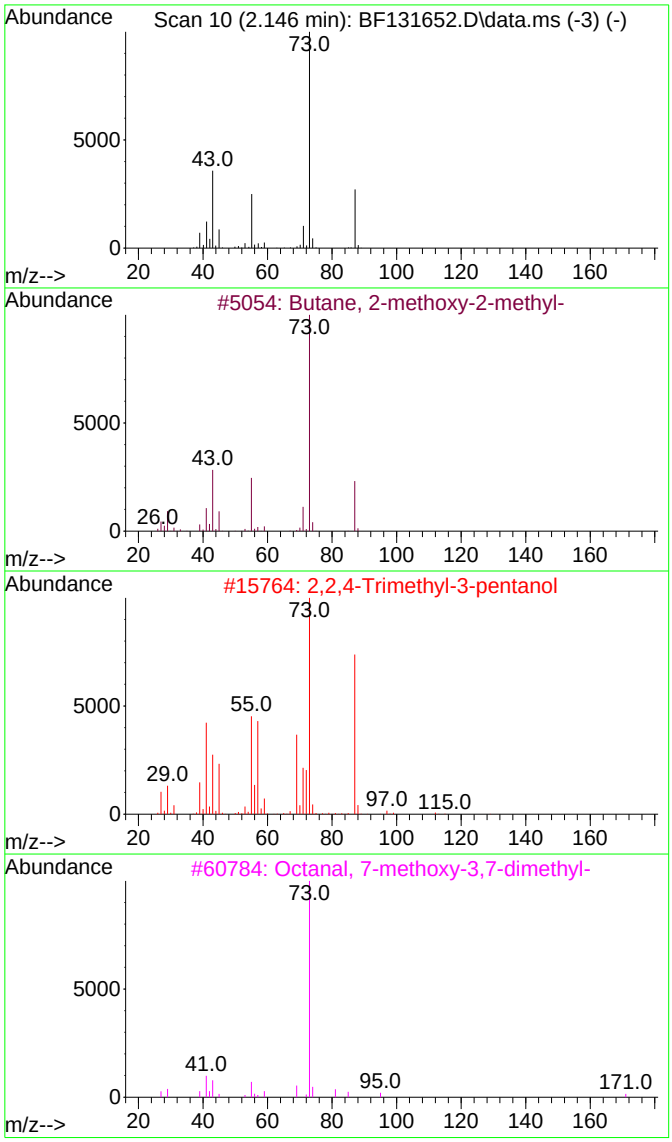
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

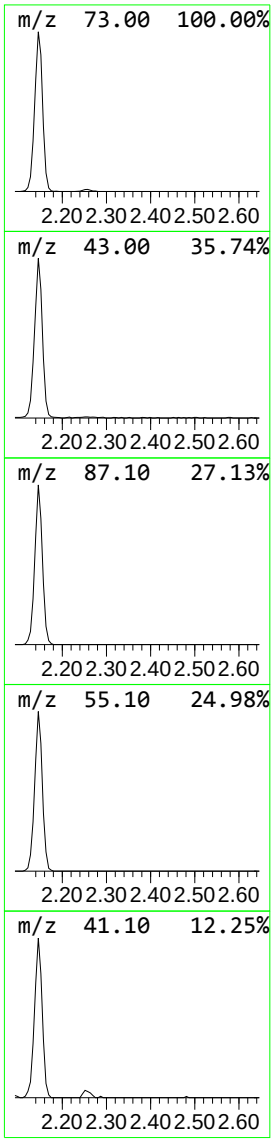
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	27.44 ng	516600	1,4-Dichlorobenzene-d4	6.881

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	39
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





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Sample : N6038-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-35-(2.5-4.5)

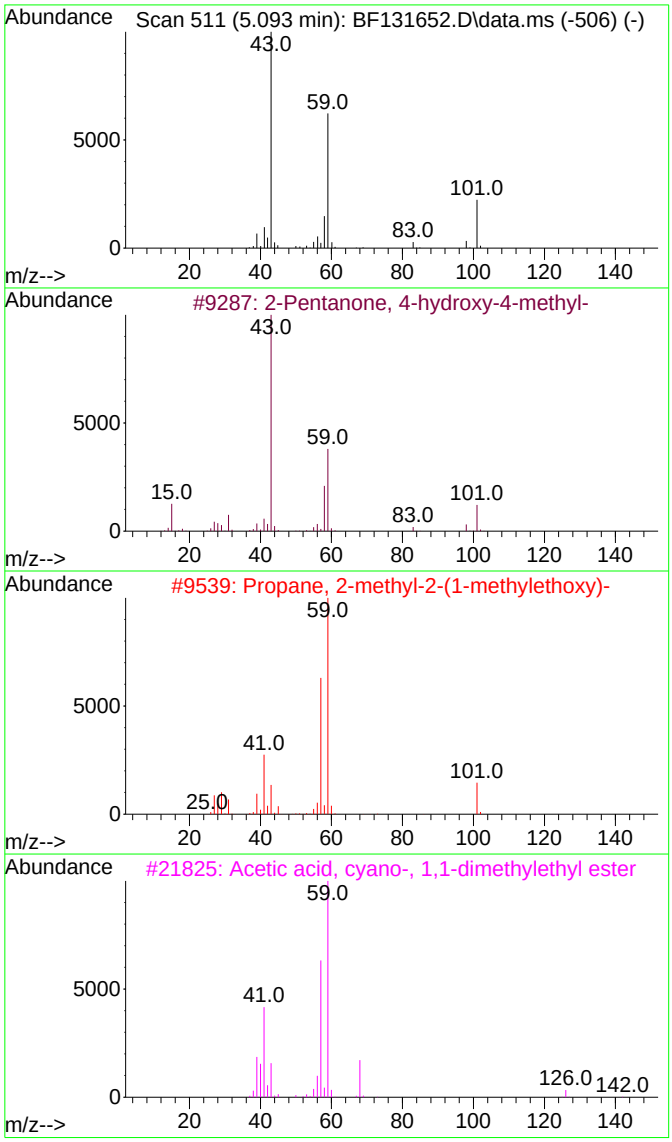
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

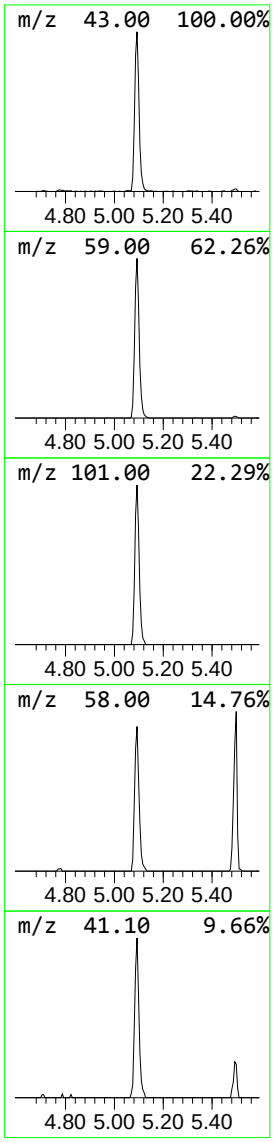
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	13.69 ng	257800	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF131652.D
Acq On : 15 Dec 2022 16:47
Operator : CG\JU
Sample : N6038-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-35-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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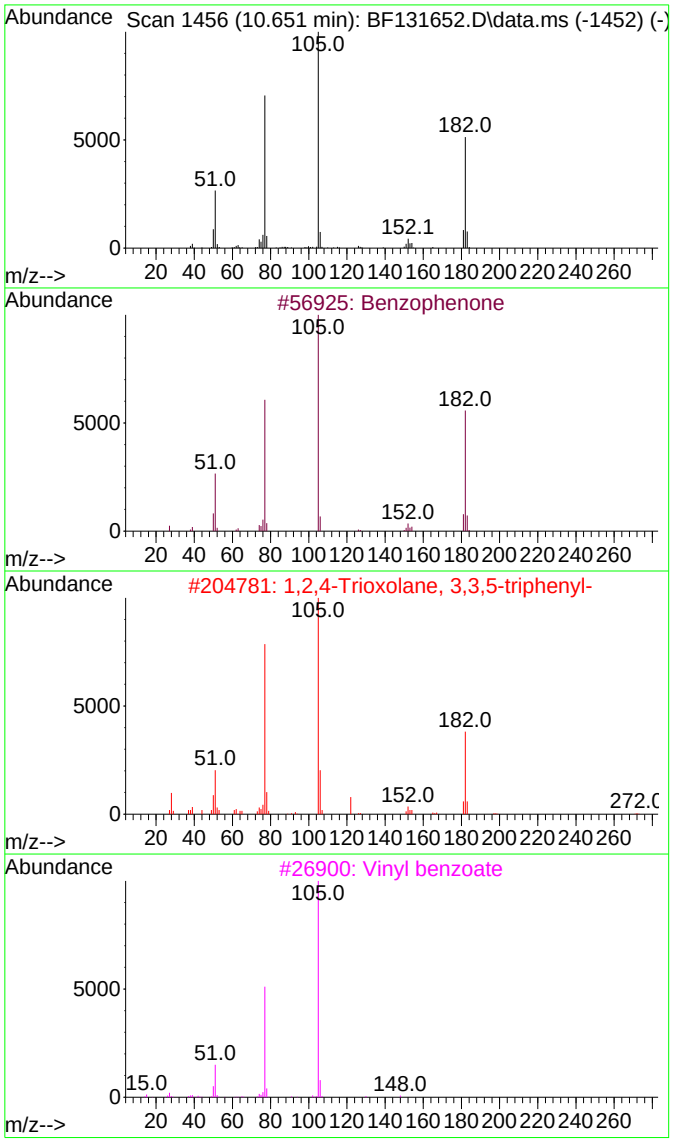
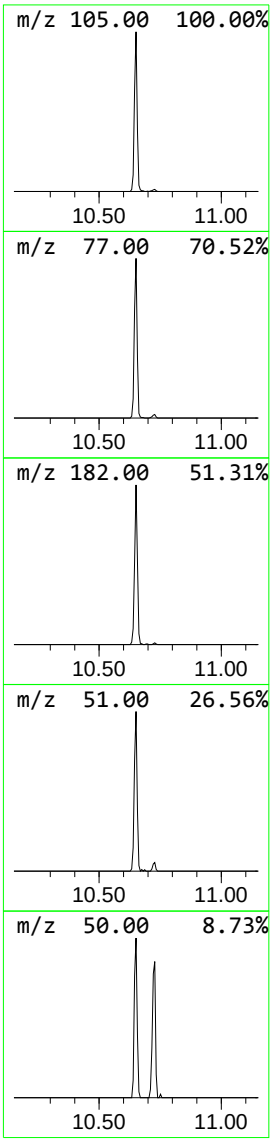
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	7.72 ng	222035	Acenaphthene-d10	9.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47





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Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-35-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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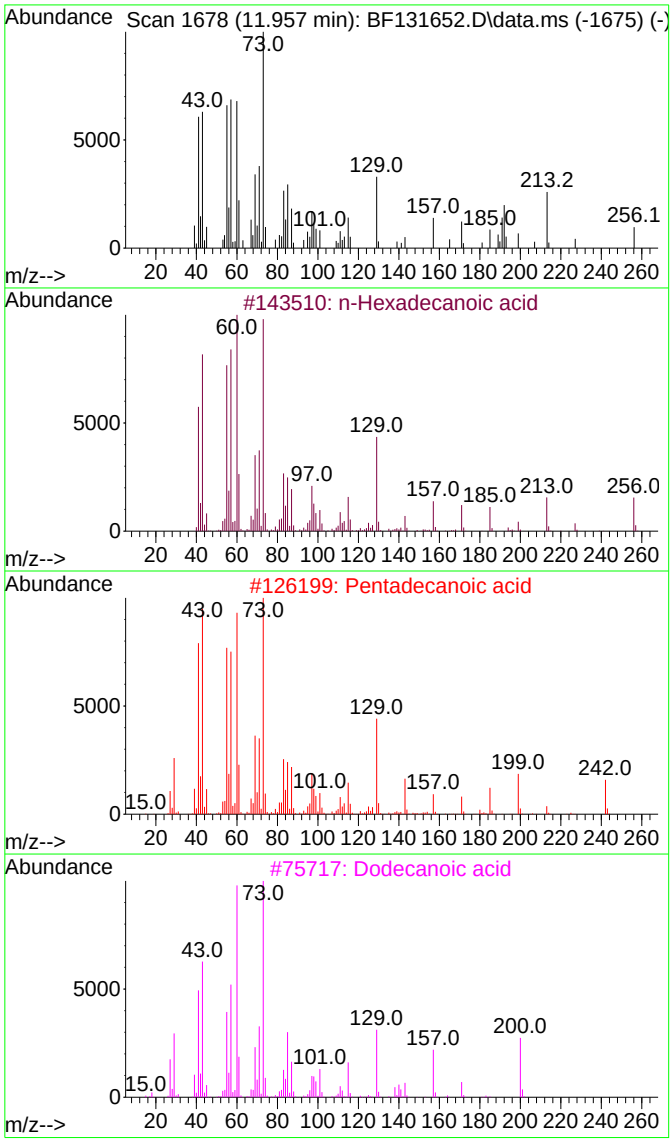
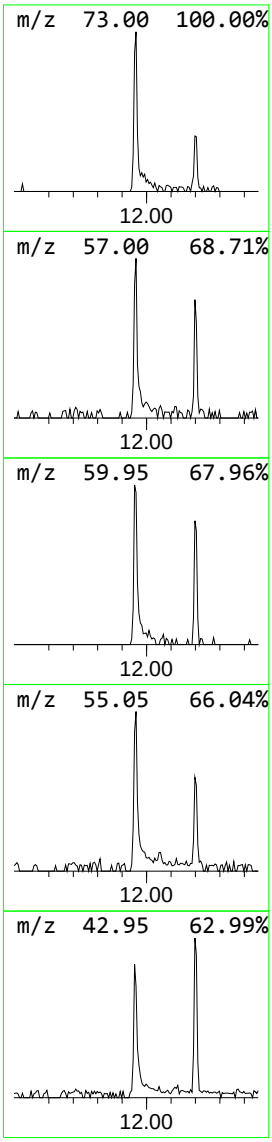
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	2.39 ng	74399	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
3	Dodecanoic acid	200	C12H24O2	000143-07-7	38
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-35-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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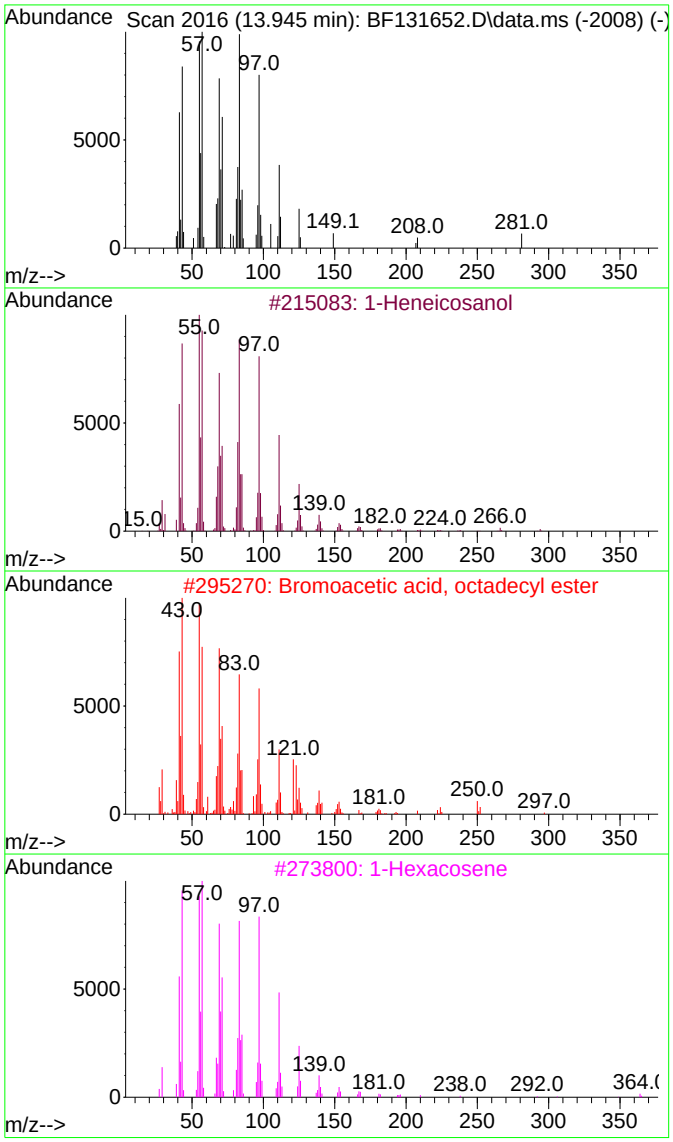
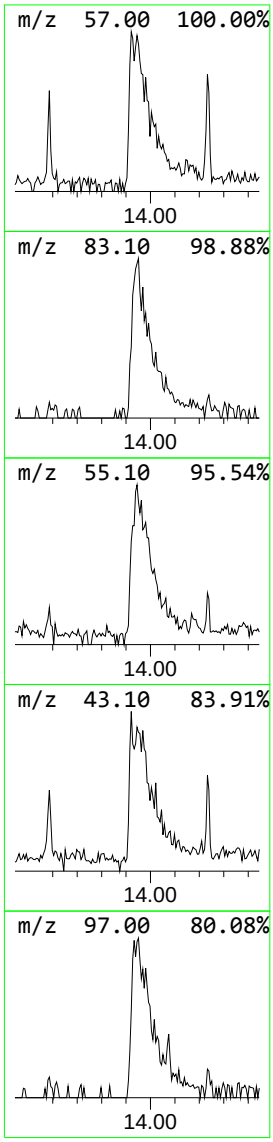
Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	8.61 ng	173310	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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RB-35-(2.5-4.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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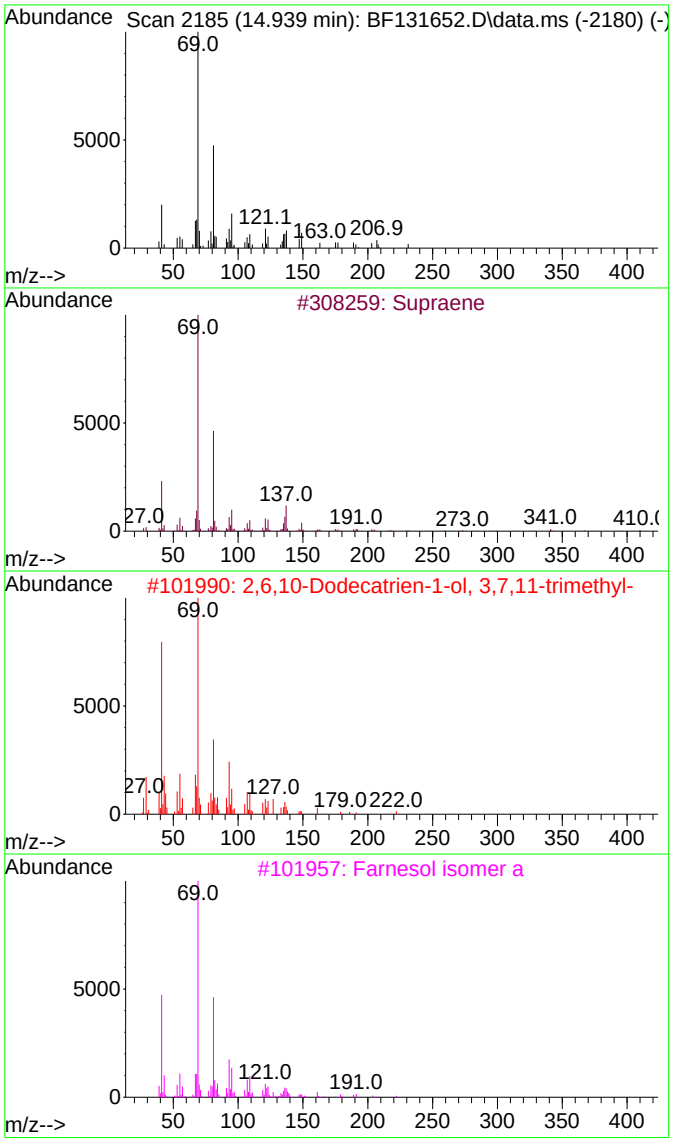
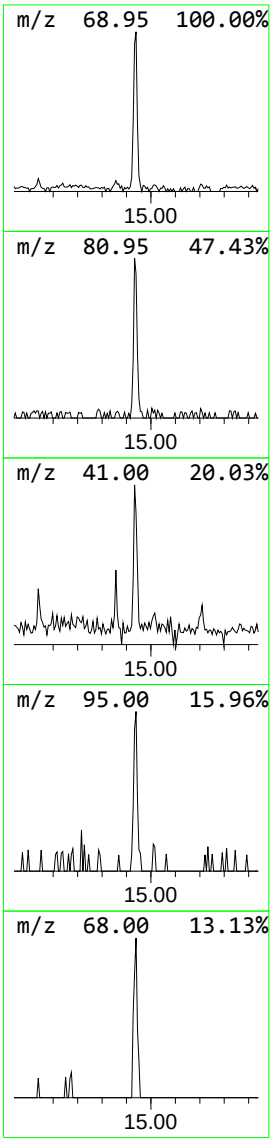
Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.25 ng	39566	Perylene-d12	15.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
3	Farnesol isomer a	222	C15H26O	1000108-92-4	64
4	Nerolidol 1	222	C15H26O	1000285-43-5	59
5	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	59





Tentatively Identified Compound (LSC) summary

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RB-35-(2.5-4.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.146	27.4	ng	516600	1	6.881	376597	20.0
2-Pentanone, 4-...	5.093	13.7	ng	257800	1	6.881	376597	20.0
Benzophenone	10.651	7.7	ng	222035	3	9.934	575054	20.0
n-Hexadecanoic ...	11.957	2.4	ng	74399	4	11.428	623369	20.0
1-Heneicosanol	13.945	8.6	ng	173310	5	14.074	402345	20.0
Supraene	14.939	2.3	ng	39566	6	15.580	351676	20.0