LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131842.D
Acq On : 27 Dec 2022 17:58
Operator : CG\JU
Sample : N6199-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-604-COMP-1

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-BF122422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	497	502	513	rVB	539758	663719	33.50%	4.415%
2	5.445	566	571	574	rBV	1807900	1613588	81.45%	10.733%
3	6.463	739	744	747	rBV	1751084	1653032	83.44%	10.996%
4	6.834	803	807	810	rBV	516219	466920	23.57%	3.106%
5	7.398	898	903	906	rBV	1143606	1108087	55.93%	7.371%
6	8.122	1021	1026	1029	rBV	698634	592113	29.89%	3.939%
7	9.204	1205	1210	1213	rBV	2391377	1981126	100.00%	13.178%
8	9.886	1321	1326	1329	rBV	810412	704251	35.55%	4.685%
9	10.604	1444	1448	1451	rBV	327754	261365	13.19%	1.739%
10	10.674	1456	1460	1464	rBV	1258870	1198475	60.49%	7.972%
11	11.380	1576	1580	1583	rBV	821226	737252	37.21%	4.904%
12	12.968	1846	1850	1854	rBV	1928617	1785153	90.11%	11.874%
13	13.880	1999	2005	2024	rBV4	46127	155322	7.84%	1.033%
14	14.027	2026	2030	2034	rBV	486334	430948	21.75%	2.867%
15	15.151	2217	2221	2226	rVB	20720	24558	1.24%	0.163%
16	15.515	2277	2283	2295	rVB	315441	450539	22.74%	2.997%
17	15.980	2356	2362	2369	rVB2	66788	105465	5.32%	0.702%
18	16.492	2443	2449	2457	rVB2	99923	175446	8.86%	1.167%
19	17.098	2545	2552	2561	rBV	124768	261299	13.19%	1.738%
20	17.809	2664	2673	2683	rVB2	126830	308867	15.59%	2.055%
21	18.656	2804	2817	2832	rBV3	113351	356080	17.97%	2.369%

Sum of corrected areas: 15033605

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
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Misc :
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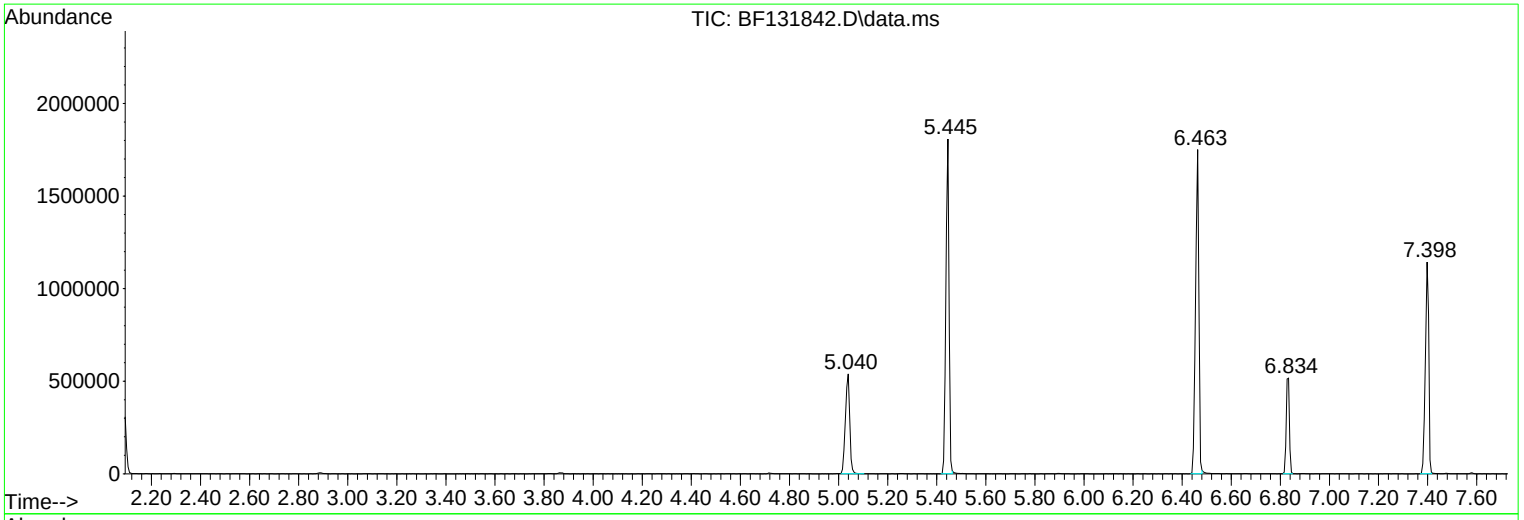
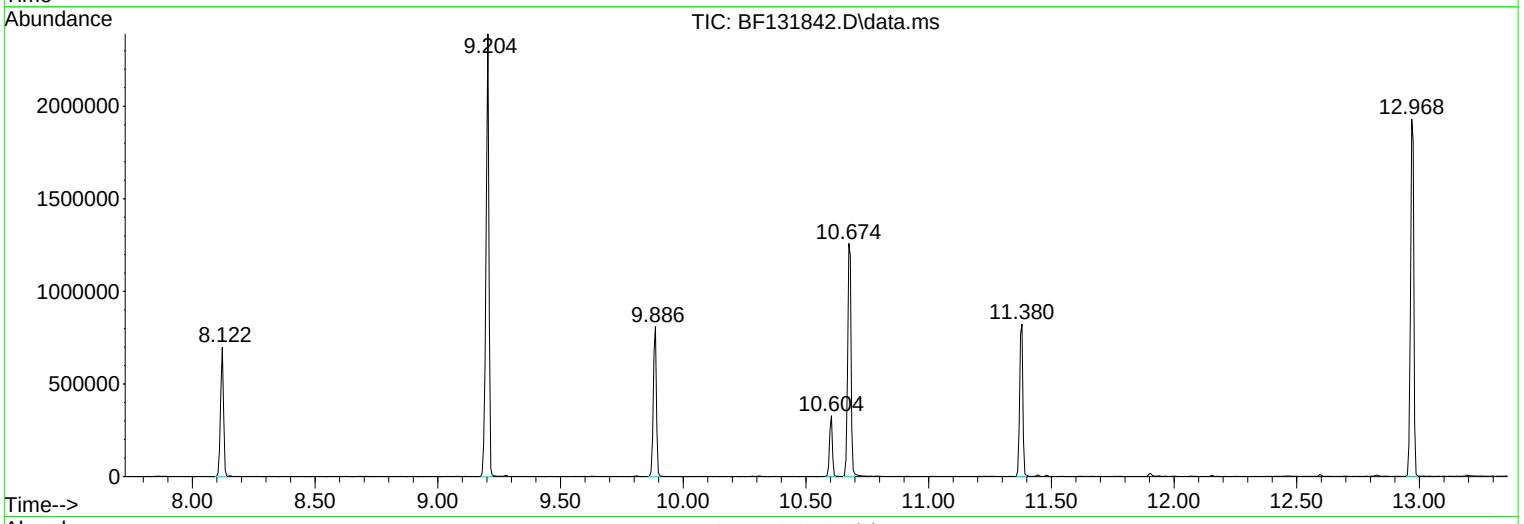
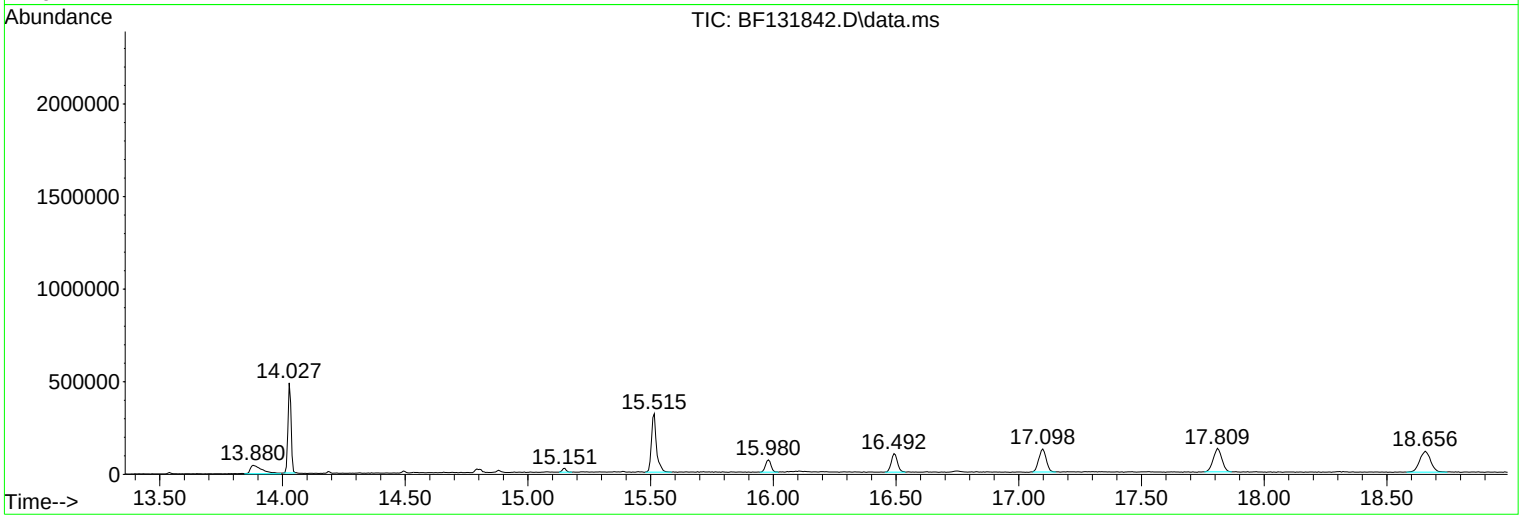
Instrument :
BNA_F
ClientSampleId :
TR-604-COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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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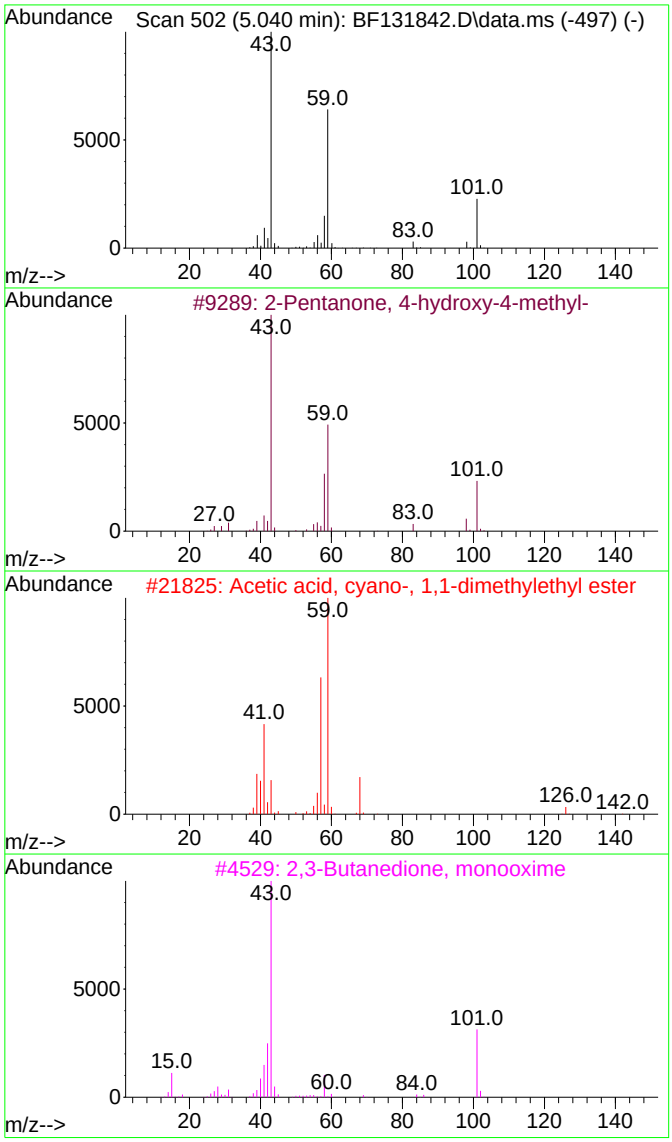
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

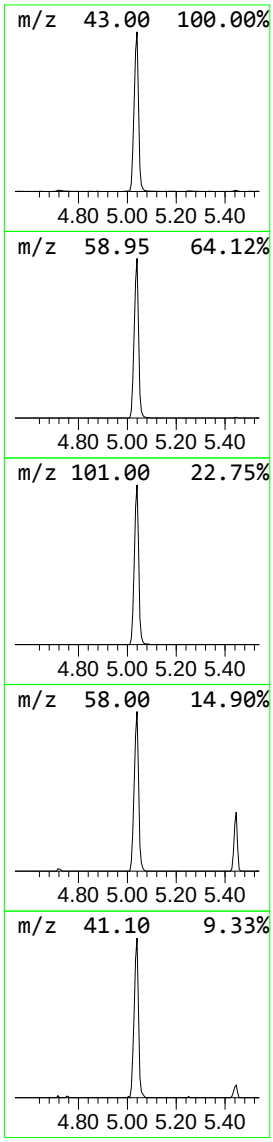
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	28.43 ng	663719	1,4-Dichlorobenzene-d4	6.834

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF131842.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

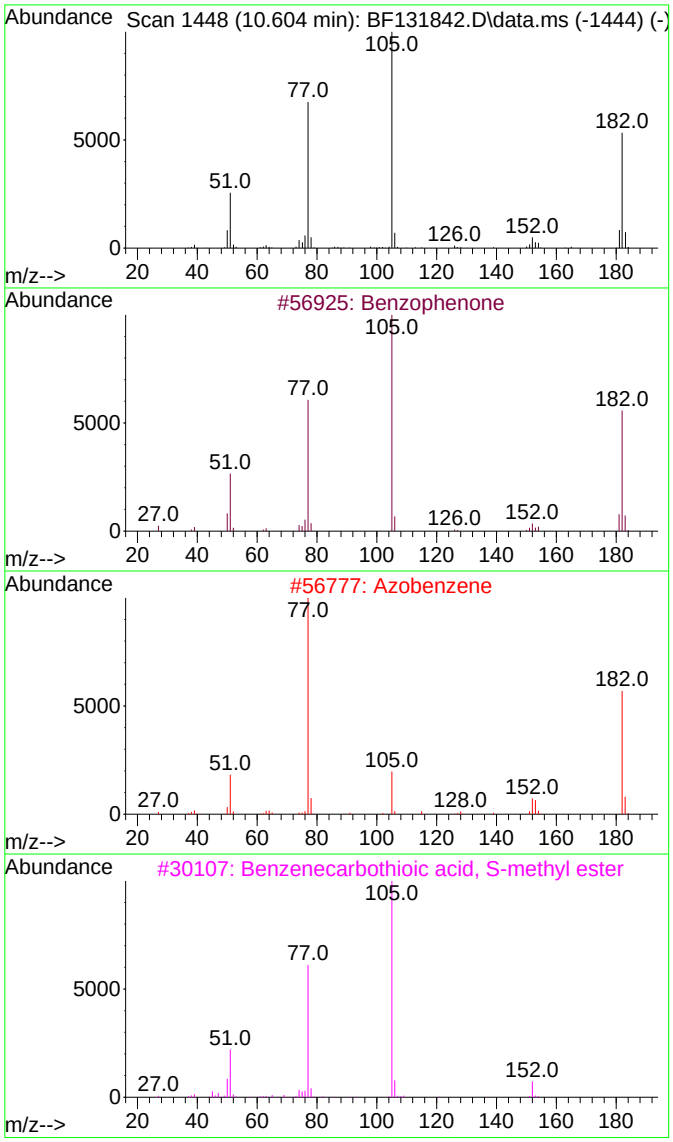
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

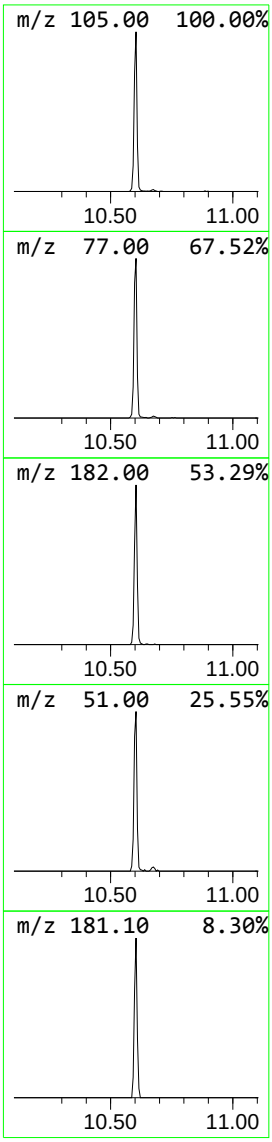
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	7.42 ng	261365	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Operator : CG\JU
Sample : N6199-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
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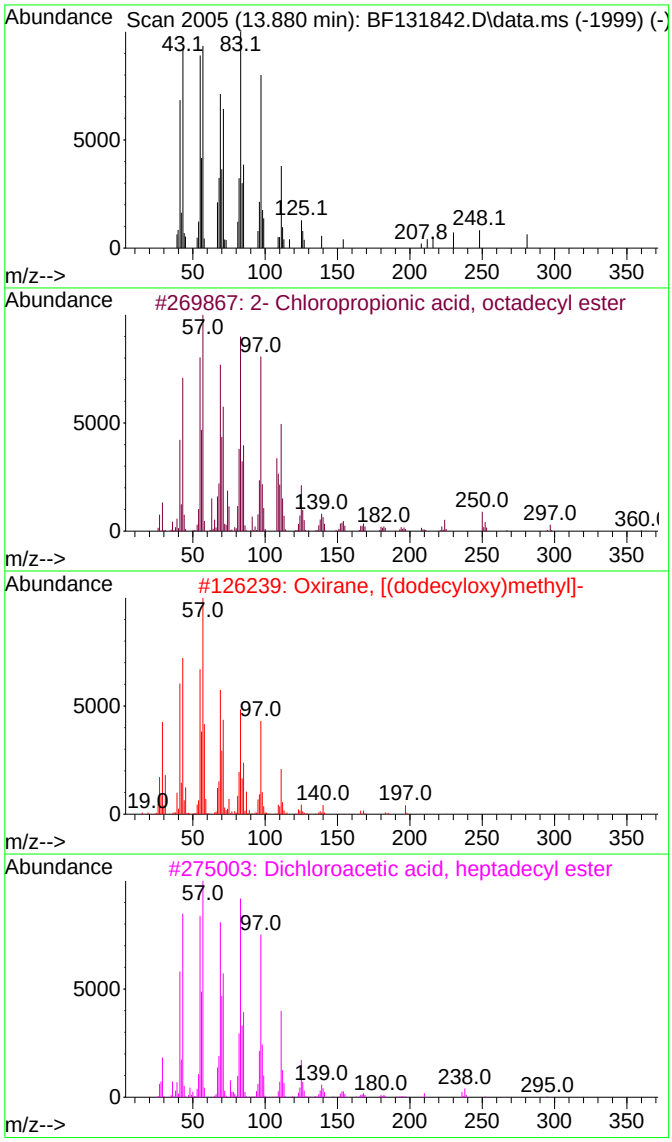
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

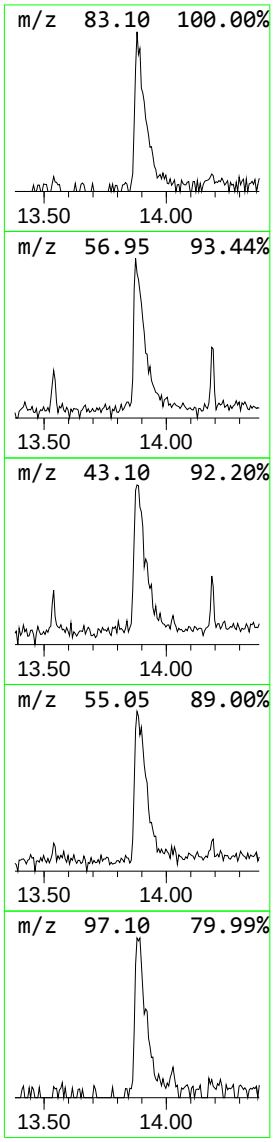
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2- Chloropropionic acid, oc... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	7.21 ng	155322	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4	1-Octadecanol	270	C18H38O	000112-92-5	81
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81





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ClientSampleId :
TR-604-COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

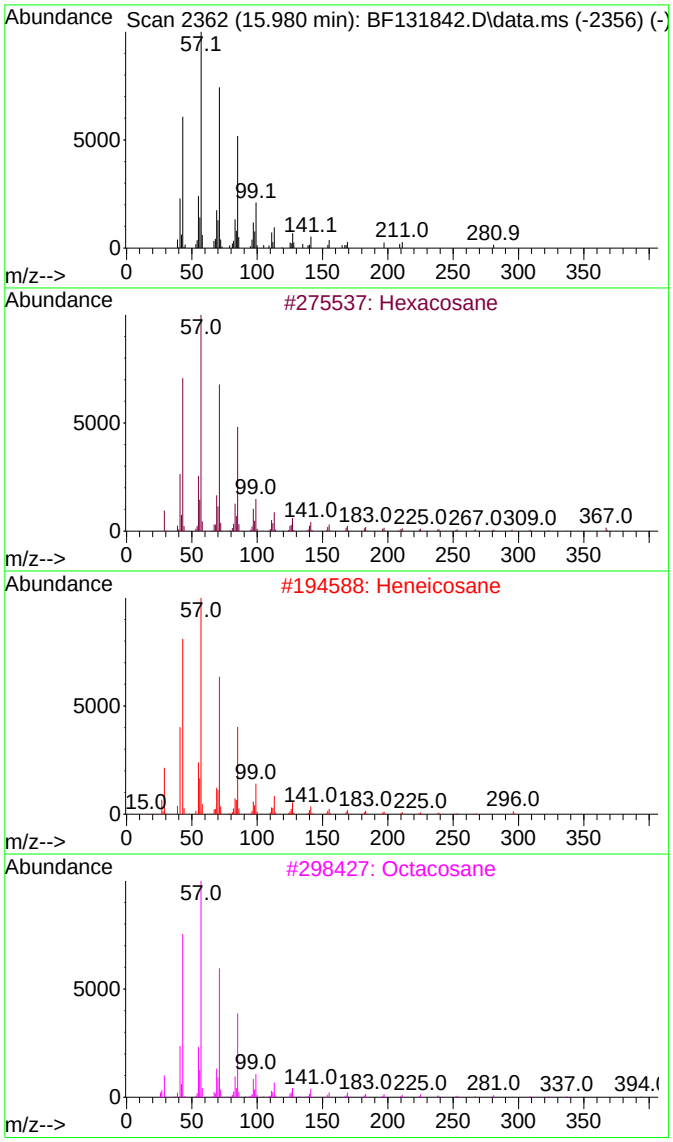
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

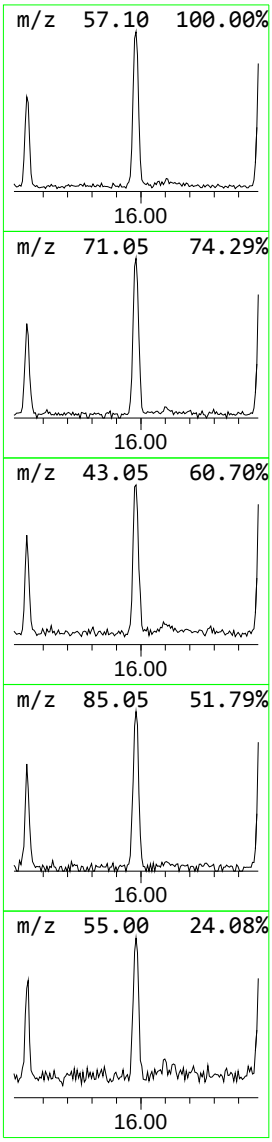
****

Peak Number 4 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	4.68 ng	105465	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Nonadecane	268	C19H40	000629-92-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131842.D
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Operator : CG\JU
Sample : N6199-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-604-COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

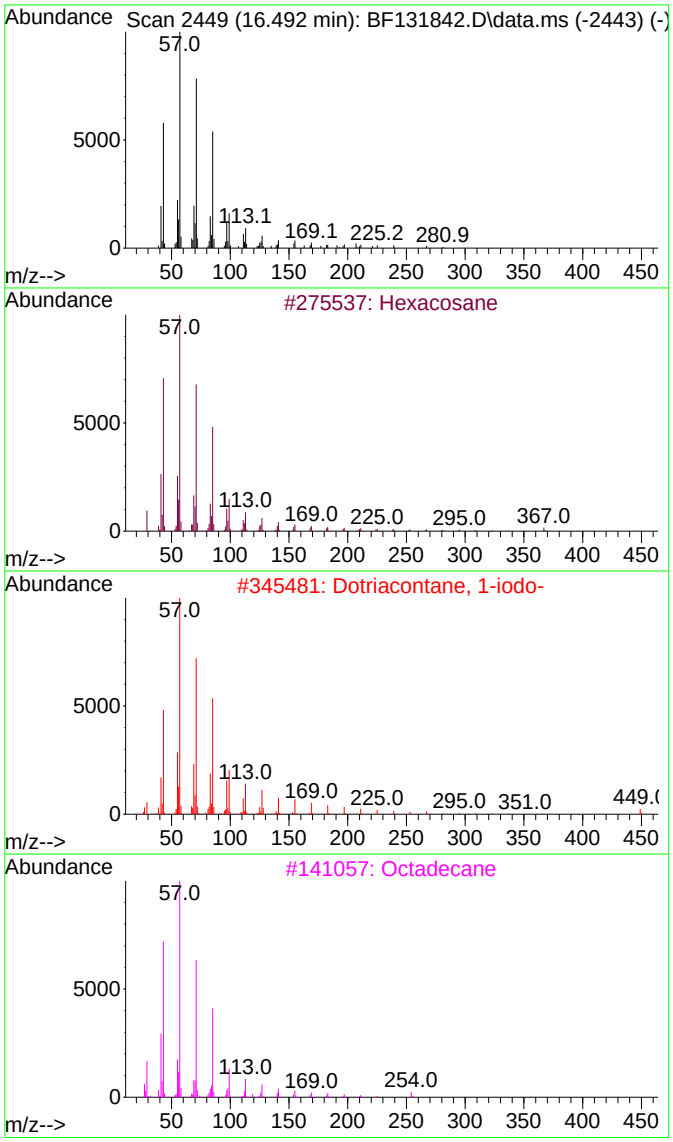
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

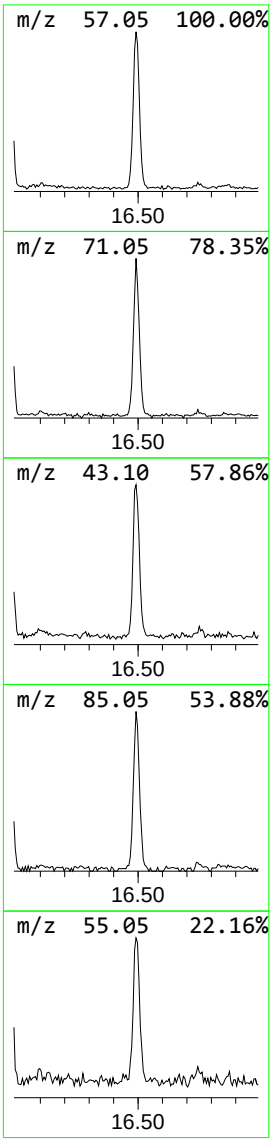
****

Peak Number 5 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	7.79 ng	175446	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
3	Octadecane	254	C18H38	000593-45-3	86
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-604-COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

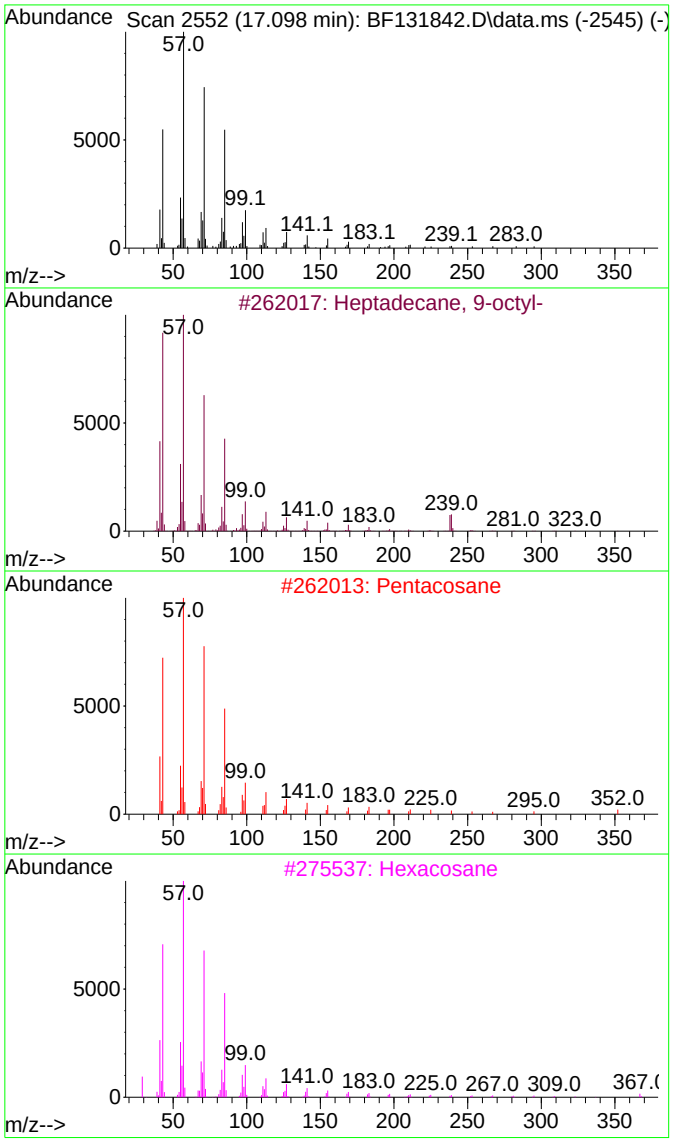
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

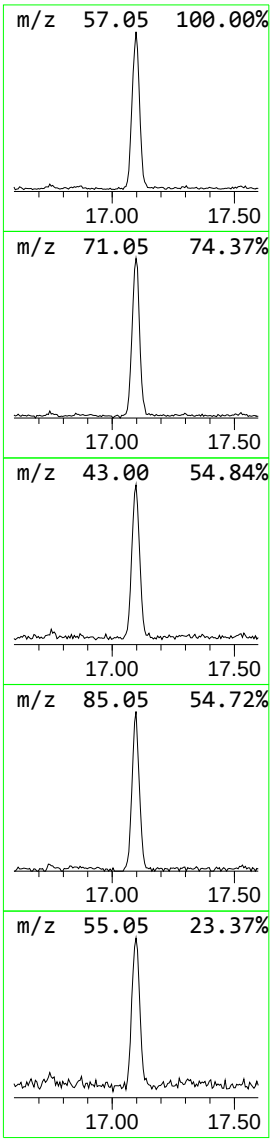
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.098	11.60 ng	261299	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-604-COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

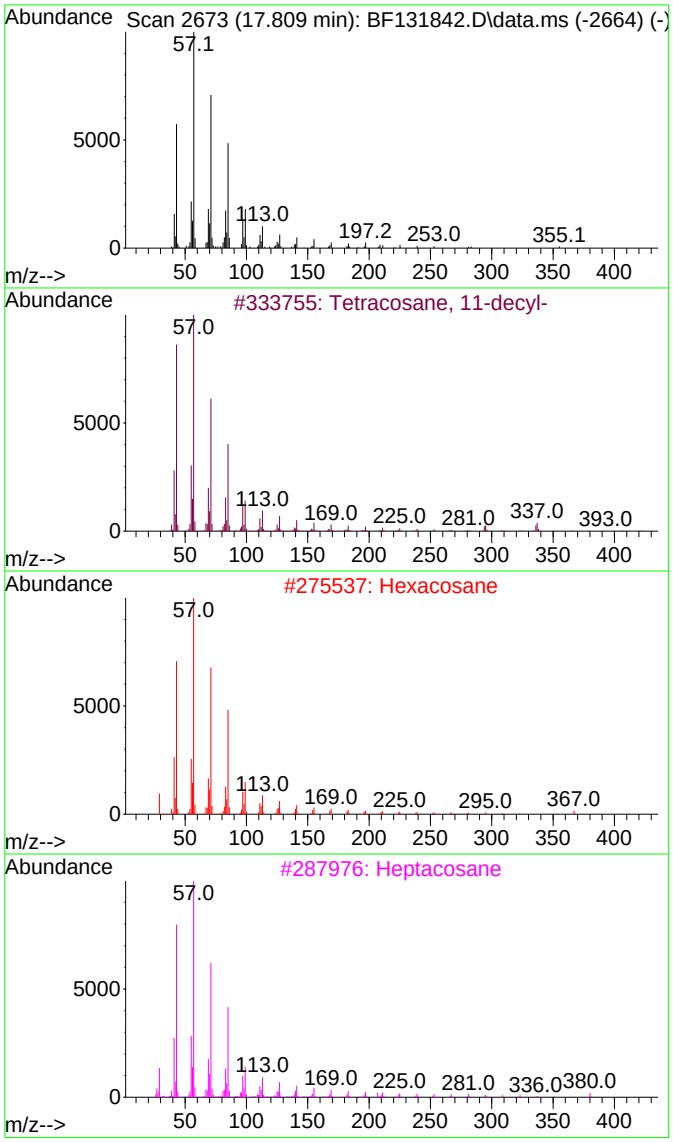
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

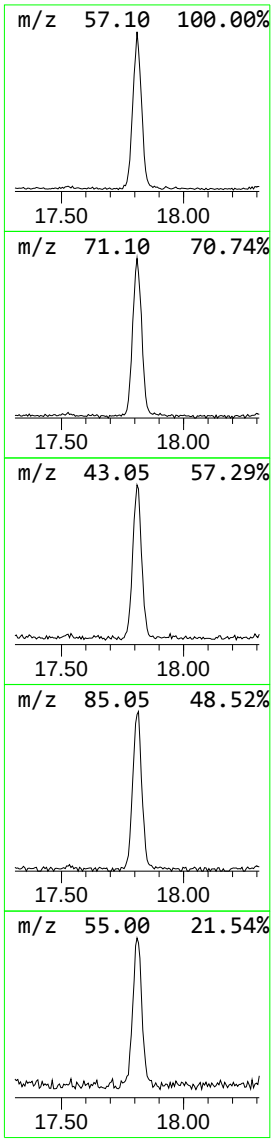
****

Peak Number 7 Tetracosane, 11-decyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.809	13.71 ng	308867	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

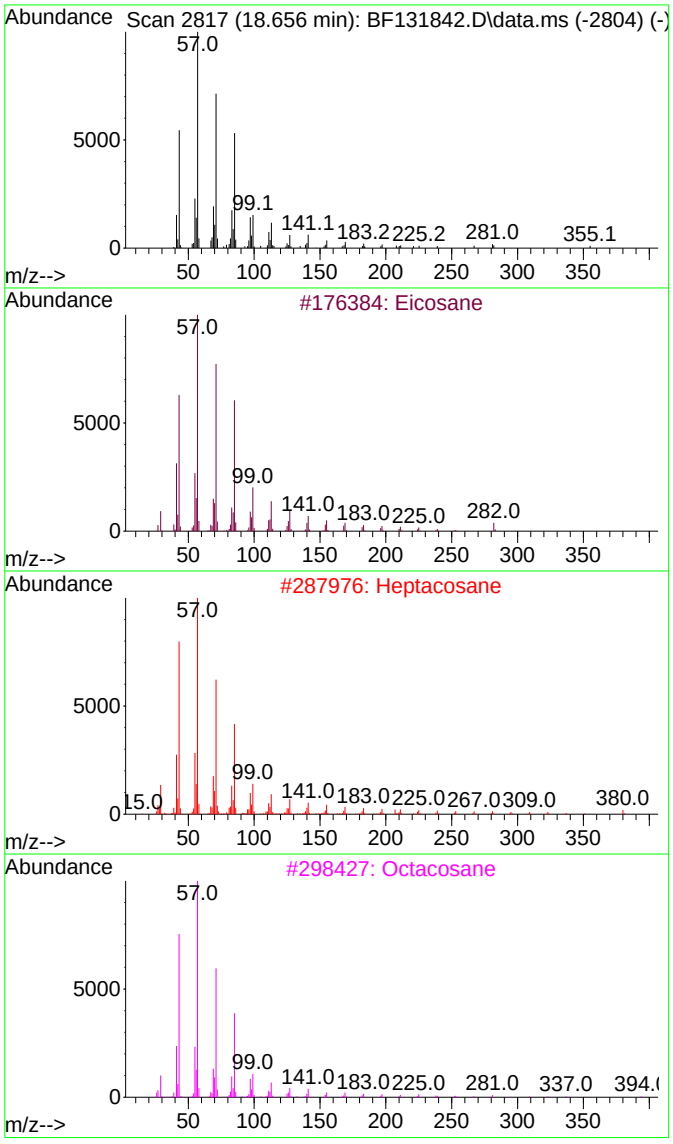
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

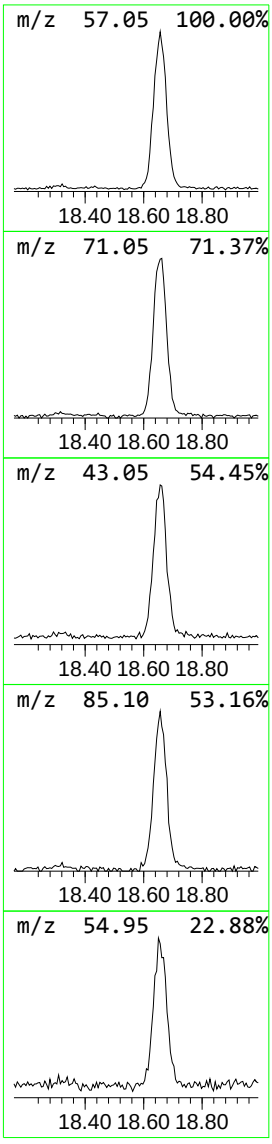
****

Peak Number 8 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.656	15.81 ng	356080	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





Tentatively Identified Compound (LSC) summary

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Data File : BF131842.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
2-Pentanone, 4-...	5.040	28.4	ng	663719	1	6.834	466920	20.0
Benzophenone	10.604	7.4	ng	261365	3	9.886	704251	20.0
2- Chloropropio...	13.880	7.2	ng	155322	5	14.027	430948	20.0
Hexacosane	15.980	4.7	ng	105465	6	15.515	450539	20.0
Dotriacontane, ...	16.492	7.8	ng	175446	6	15.515	450539	20.0
Heptadecane, 9-...	17.098	11.6	ng	261299	6	15.515	450539	20.0
Tetracosane, 11...	17.809	13.7	ng	308867	6	15.515	450539	20.0
Eicosane	18.656	15.8	ng	356080	6	15.515	450539	20.0