LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118619.D
Acq On : 21 Jan 2020 5:44
Operator : CG/JU
Sample : PB126132BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126132BL

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-BF012020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	15	24	33	rVB	2102360	3003985	24.34%	2.878%
2	5.116	507	515	524	rBV	1751114	2551043	20.67%	2.444%
3	5.516	577	583	586	rBV	9600304	11030980	89.39%	10.567%
4	6.516	746	753	762	rBV	9681293	11515987	93.32%	11.031%
5	6.657	771	777	780	rBV	11033285	11647187	94.39%	11.157%
6	6.881	812	815	819	rBV	2843707	2428565	19.68%	2.326%
7	7.045	838	843	846	rVB	9311235	9474577	76.78%	9.076%
8	7.439	904	910	914	rBV	6271537	7126781	57.75%	6.827%
9	8.163	1029	1033	1037	rBV	3277916	2827256	22.91%	2.708%
10	9.245	1211	1217	1220	rBV	11968376	12339729	100.00%	11.820%
11	9.628	1278	1282	1286	rBV	505017	426937	3.46%	0.409%
12	9.922	1326	1332	1335	rBV	3348359	2785411	22.57%	2.668%
13	10.710	1461	1466	1469	rBV	6770305	6321434	51.23%	6.055%
14	11.404	1580	1584	1588	rBV	2841913	2351900	19.06%	2.253%
15	11.927	1670	1673	1677	rBV	169555	170961	1.39%	0.164%
16	12.992	1849	1854	1857	rBV	11133023	10938214	88.64%	10.478%
17	13.886	2002	2006	2013	rBV	1017099	1089823	8.83%	1.044%
18	14.039	2028	2032	2036	rBV	2324829	2214190	17.94%	2.121%
19	14.210	2058	2061	2065	rBV	185578	186184	1.51%	0.178%
20	14.515	2110	2113	2117	rVB	312278	283039	2.29%	0.271%
21	14.827	2162	2166	2171	rVB	460650	469166	3.80%	0.449%
22	14.904	2176	2179	2184	rVB	215914	229641	1.86%	0.220%
23	15.168	2220	2224	2232	rBV	399770	516925	4.19%	0.495%
24	15.515	2278	2283	2287	rBV	1398857	1722338	13.96%	1.650%
25	15.557	2287	2290	2295	rVB	390255	482806	3.91%	0.462%
26	16.004	2362	2366	2370	rVB	190193	259268	2.10%	0.248%

Sum of corrected areas: 104394327

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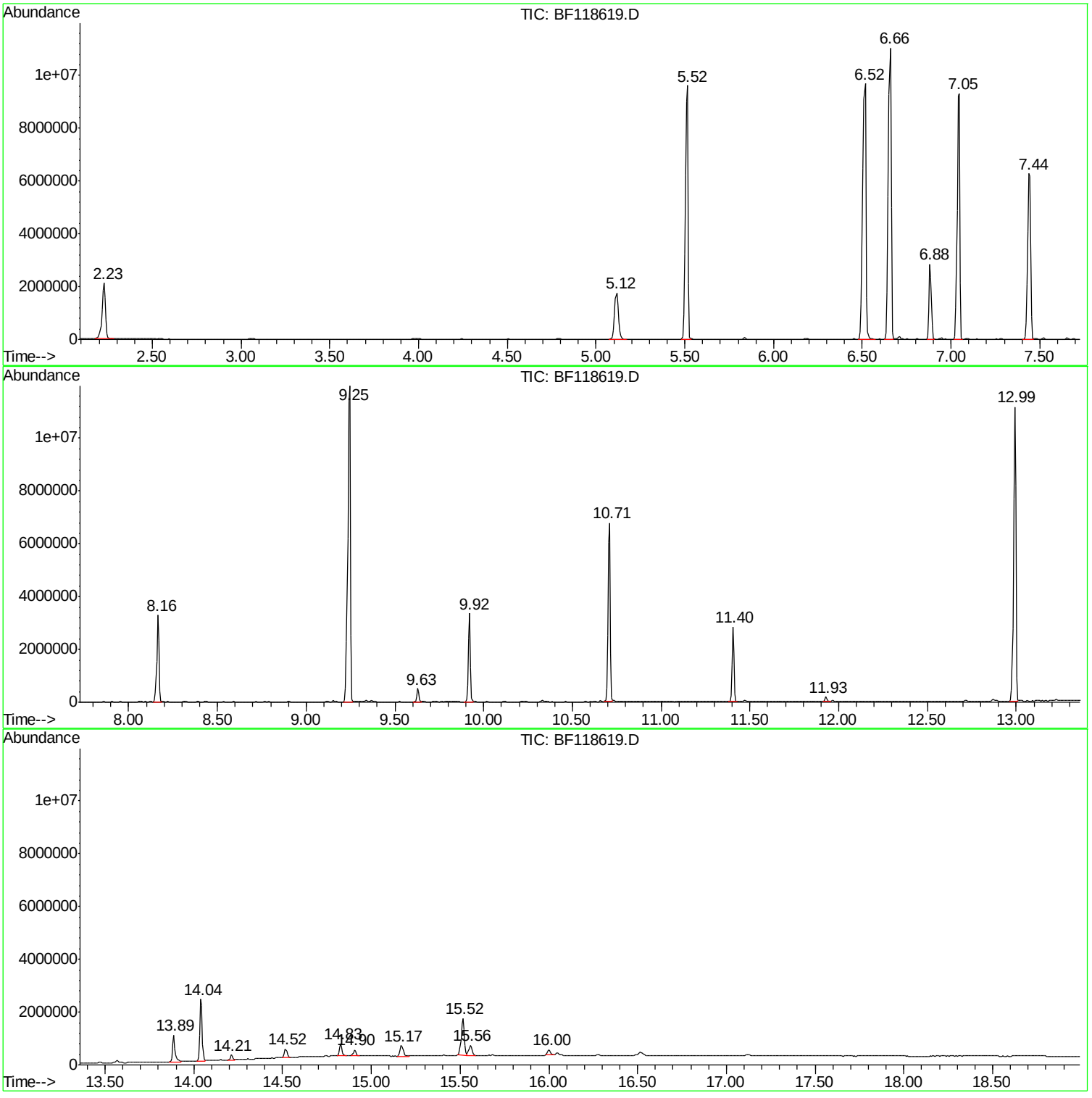
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126132BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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ClientSampleId : PB126132BL

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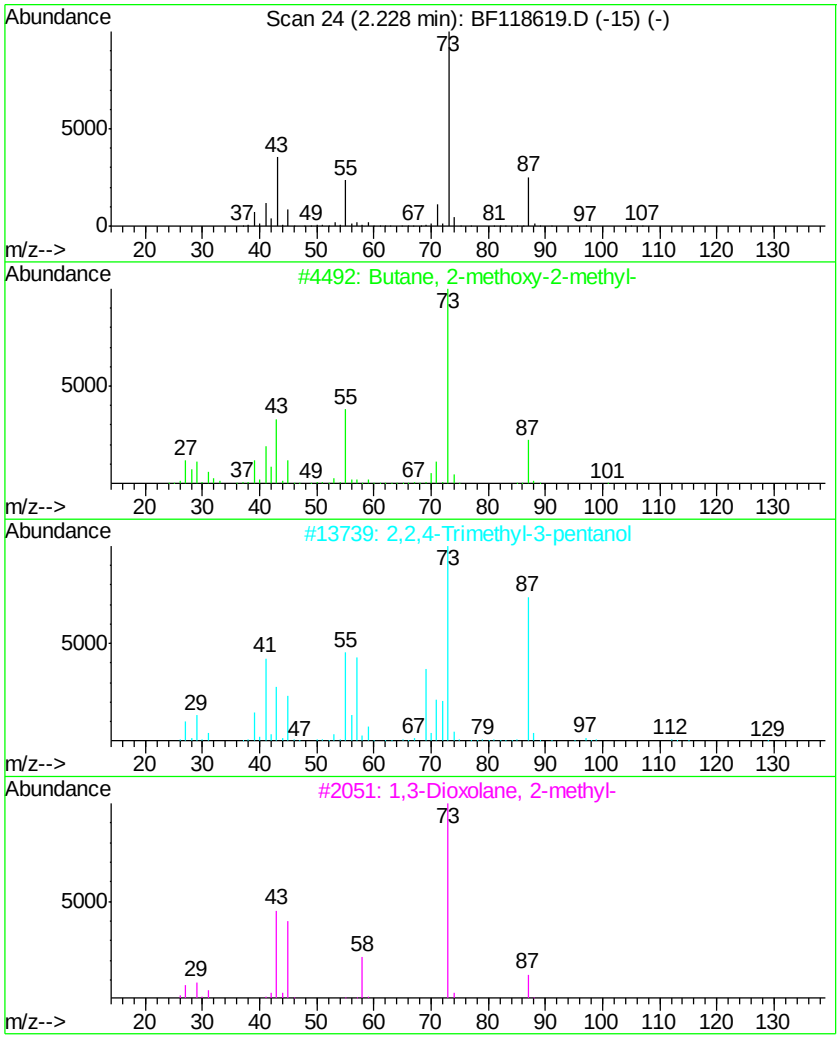
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

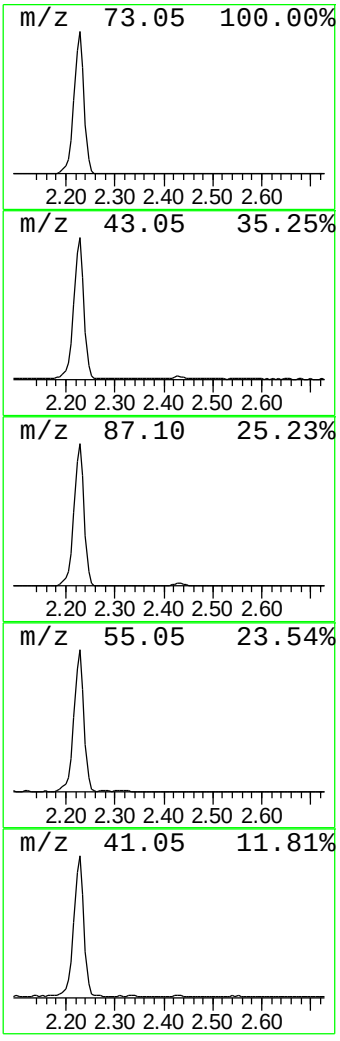
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	24.74 ng	3003990	1,4-Dichlorobenzene-d4	6.88

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : CG/JU
Sample : PB126132BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB126132BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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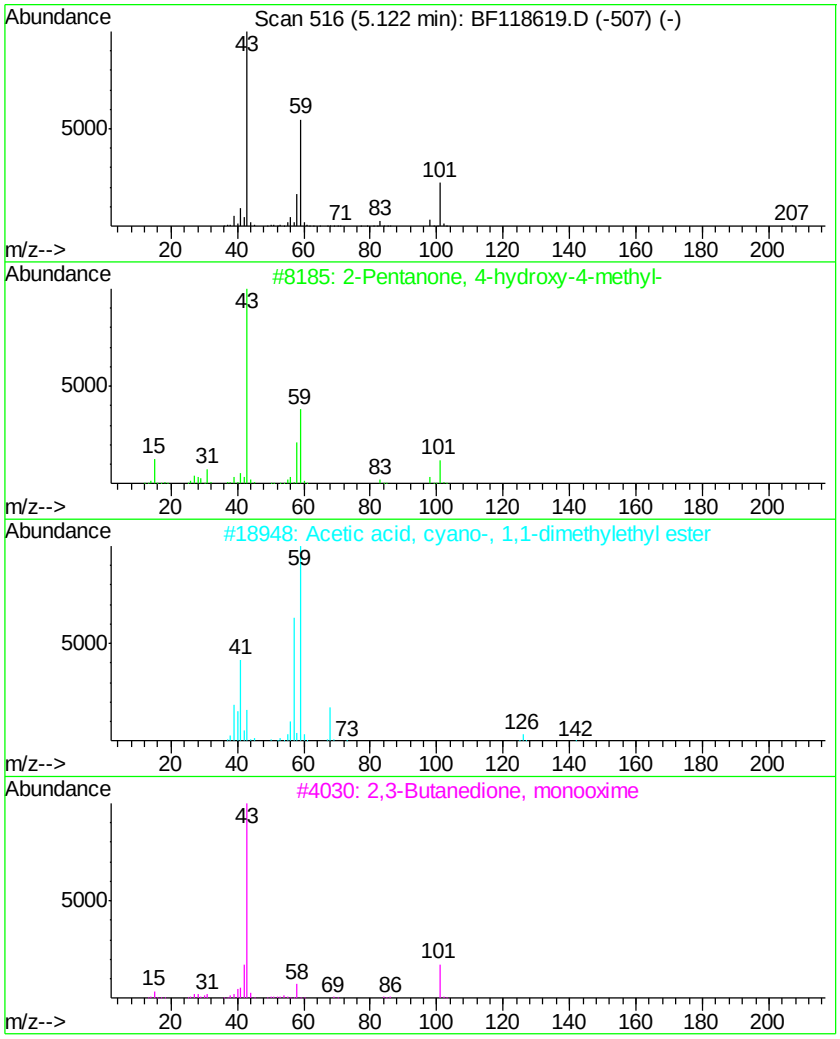
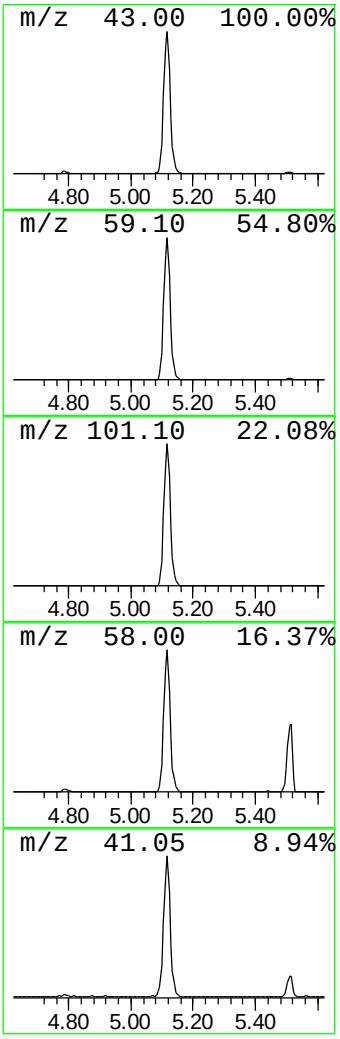
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	21.01 ng	2551040	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Acq On : 21 Jan 2020 5:44
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Sample : PB126132BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126132BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
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TIC Library : C:\DATABASE\NIST11.L
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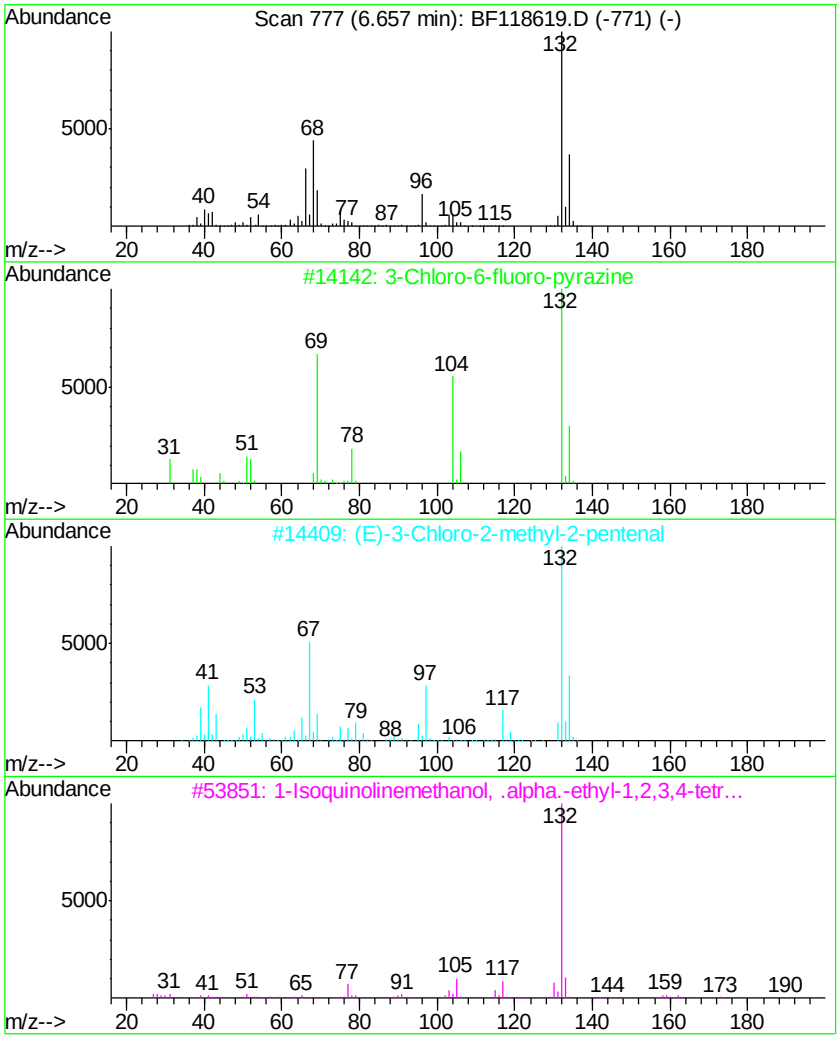
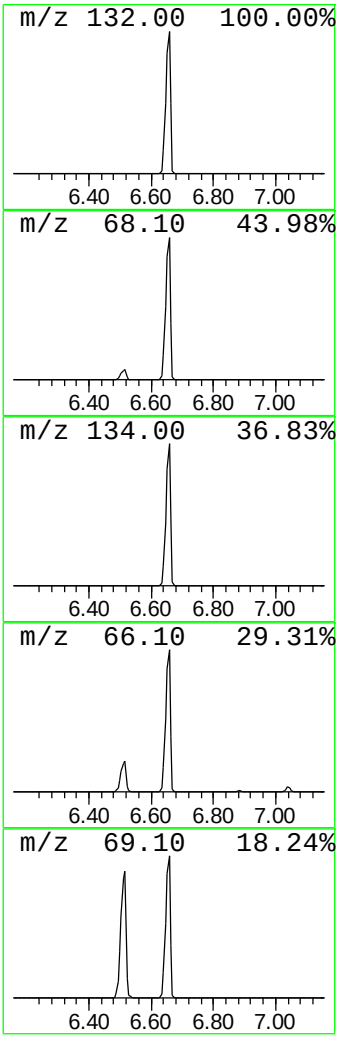
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	95.92 ng	11647200	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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TIC Library : C:\DATABASE\NIST11.L
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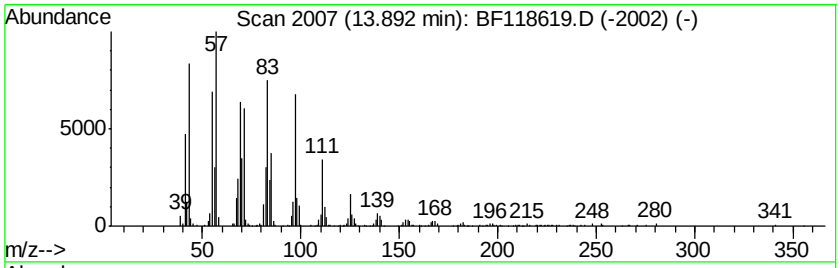
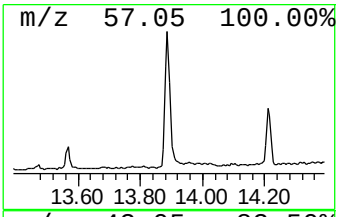
****

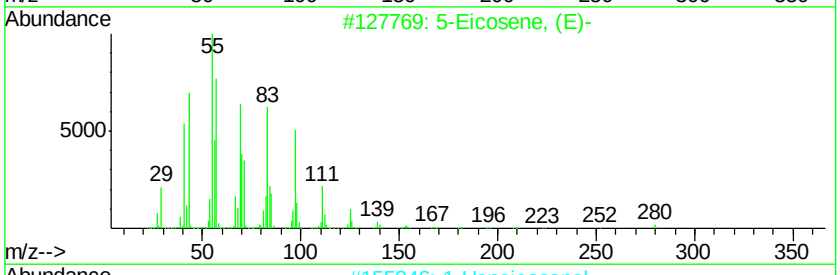
Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

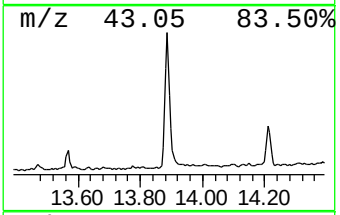
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	9.84 ng	1089820	Chrysene-d12	14.04

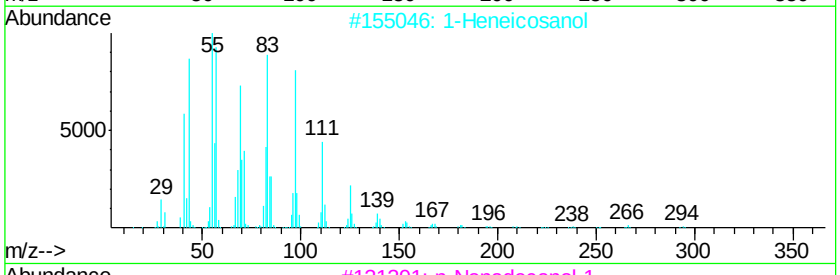
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94

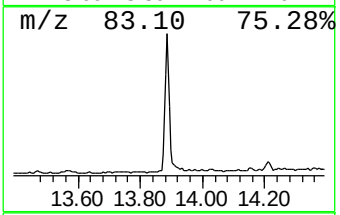


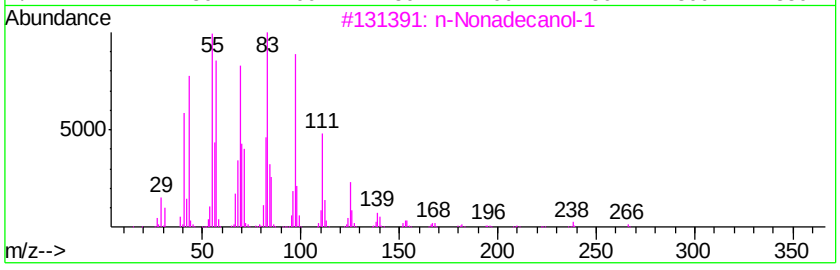


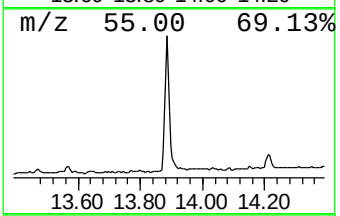


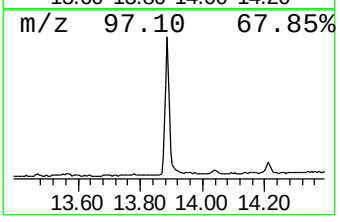












Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

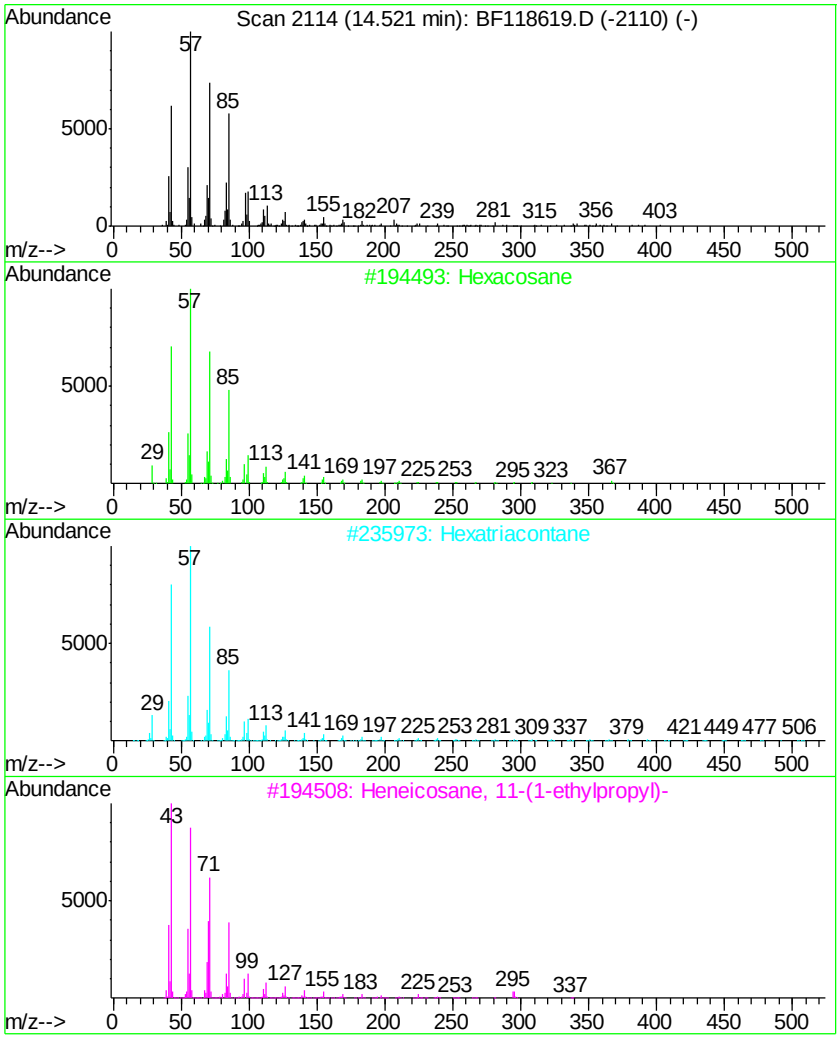
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

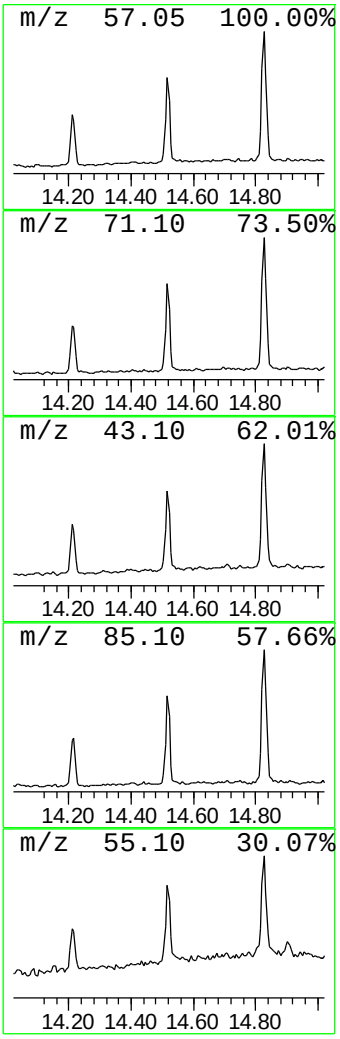
****

Peak Number 6 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.56 ng	283039	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	2-methylhexacosane	380	C27H56	1000376-72-7	91
5	10-Methylnonadecane	282	C20H42	056862-62-5	91





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

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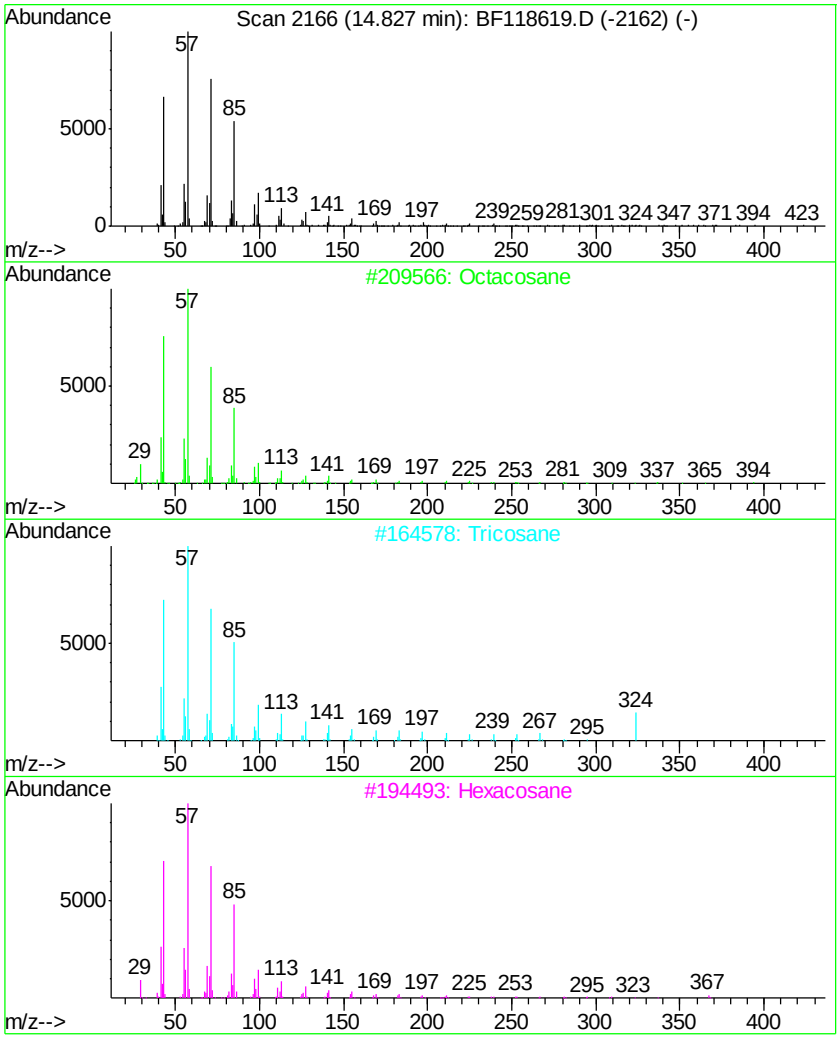
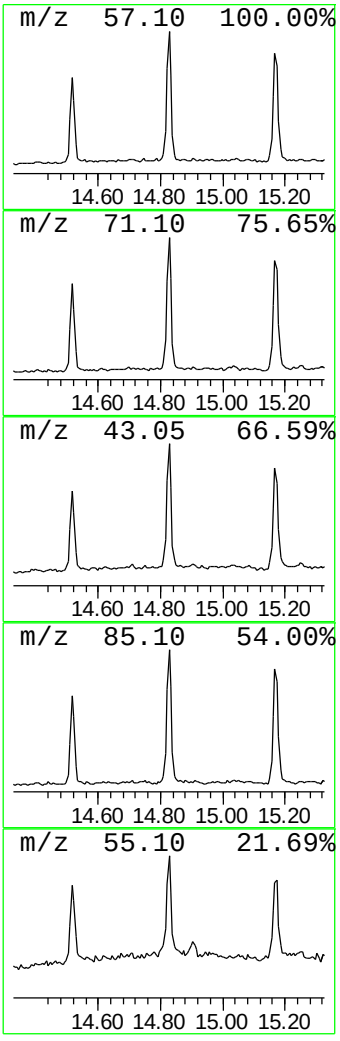
Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	5.45 ng	469166	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	96
2	Tricosane	324	C23H48	000638-67-5	95
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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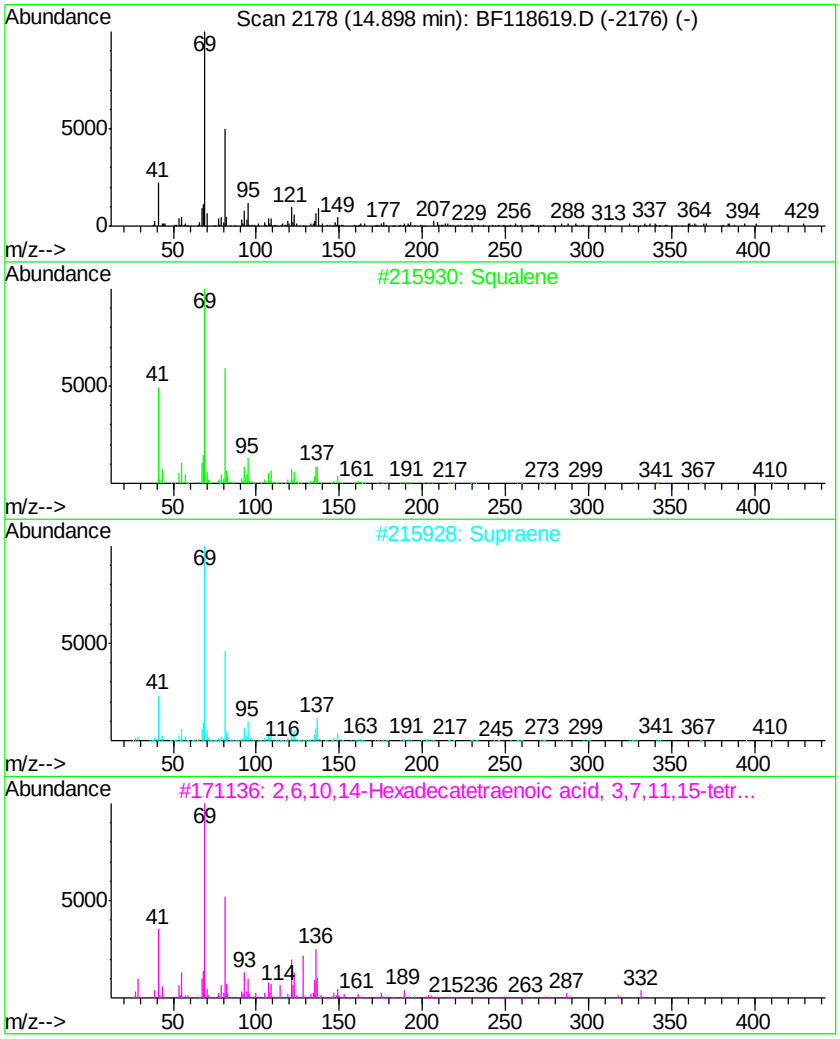
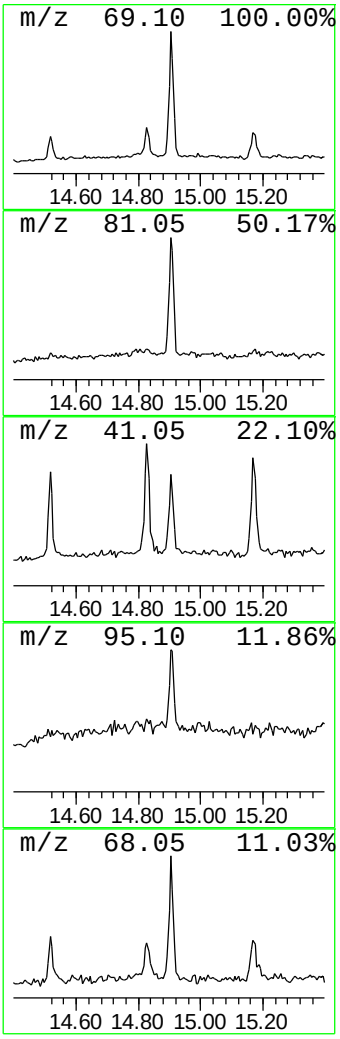
Peak Number 8 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.67 ng	229641	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	99
2	Supraene	410	C30H50	007683-64-9	94
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	81
4	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	50





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

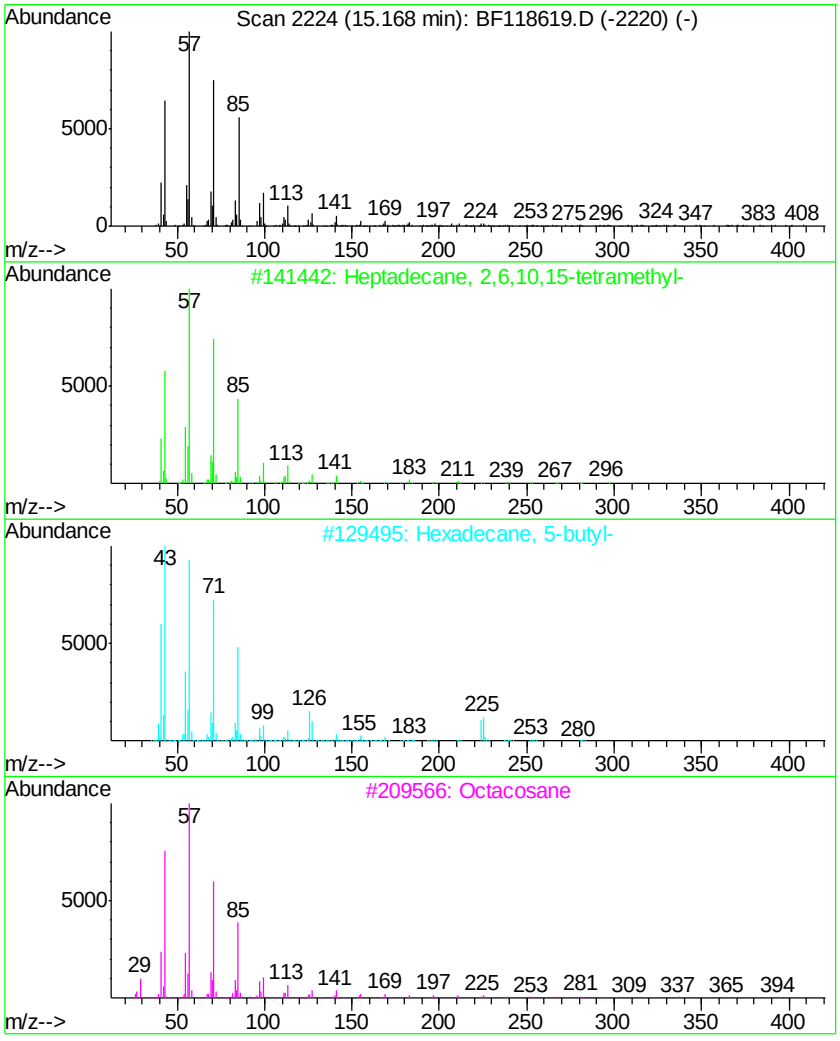
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

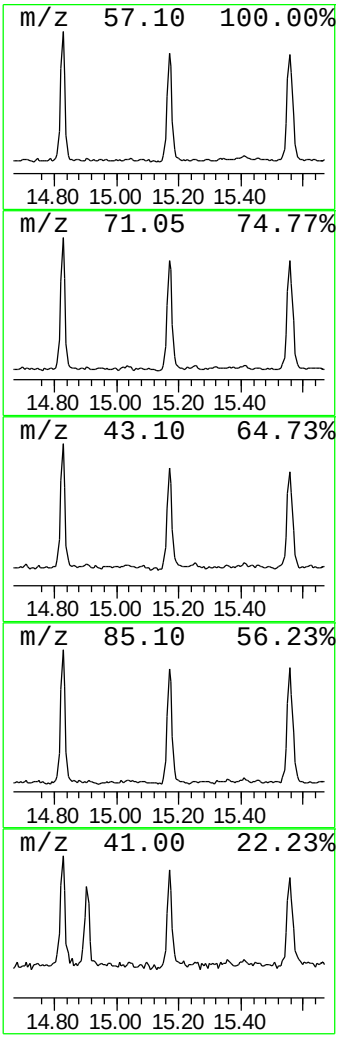
****

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	6.00 ng	516925	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	96
2	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Instrument : BNA_F
ClientSampleId : PB126132BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

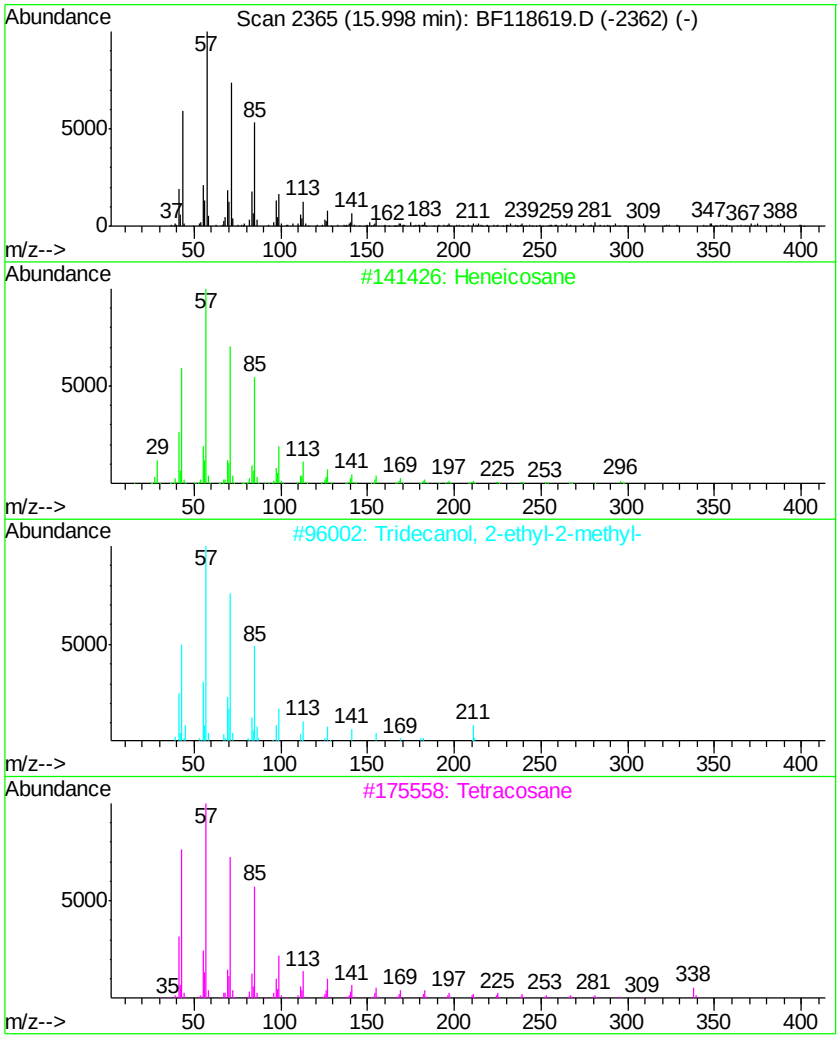
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

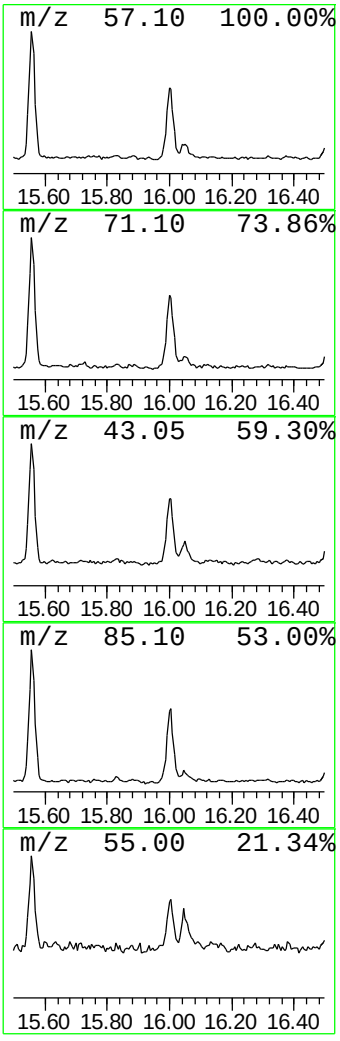
****

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	3.01 ng	259268	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
Data File : BF118619.D
Acq On : 21 Jan 2020 5:44
Operator : CG/JU
Sample : PB126132BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126132BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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-methoxy...	2.23	24.7	ng	3003990	1	6.88	2428570	20.0
2-Pentanone, 4-hy...	5.12	21.0	ng	2551040	1	6.88	2428570	20.0
unknown6.66	6.66	95.9	ng	11647200	1	6.88	2428570	20.0
5-Eicosene, (E)-	13.89	9.8	ng	1089820	5	14.04	2214190	20.0
Hexacosane	14.52	2.6	ng	283039	5	14.04	2214190	20.0
Octacosane	14.83	5.5	ng	469166	6	15.52	1722340	20.0
Squalene	14.90	2.7	ng	229641	6	15.52	1722340	20.0
Heptadecane, 2,6,...	15.17	6.0	ng	516925	6	15.52	1722340	20.0
Heneicosane	16.00	3.0	ng	259268	6	15.52	1722340	20.0